



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:10 AM UTC

PDB ID : 9LNL / pdb_00009lnl
Title : Crystal structure of T2R-TTL-YQVB15 complex
Authors : Wu, C.Y.; Wang, Y.X.; Chen, Q.F.
Deposited on : 2025-01-21
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

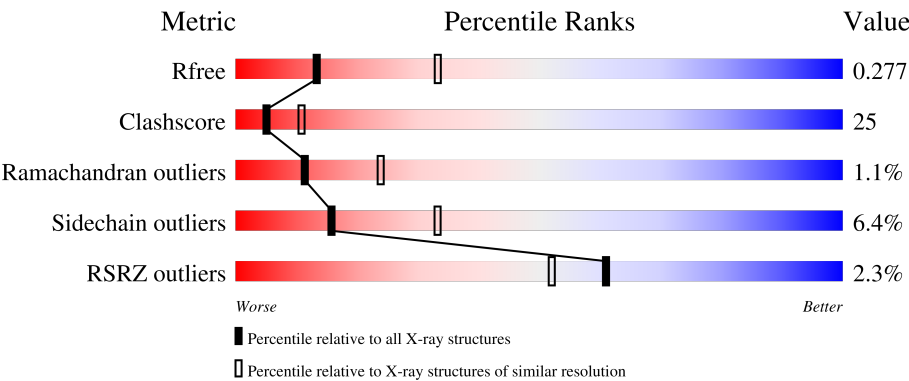
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	55% 40% ..
1	C	450	58% 37% ..
2	B	445	60% 34% ..
2	D	445	3% 43% 47% 5% 5%
3	E	143	3% 52% 29% . 16%

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Mol	Chain	Length	Quality of chain
4	F	384	6% 43% 38% 5% 14%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17617 atoms, of which 59 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	9	0
			3465	2200	584	657	24			
1	C	440	Total	C	N	O	S	8	7	0
			3466	2197	584	662	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	6	4	0
			3343	2102	567	646	28			
2	B	428	Total	C	N	O	S	6	2	0
			3370	2118	576	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

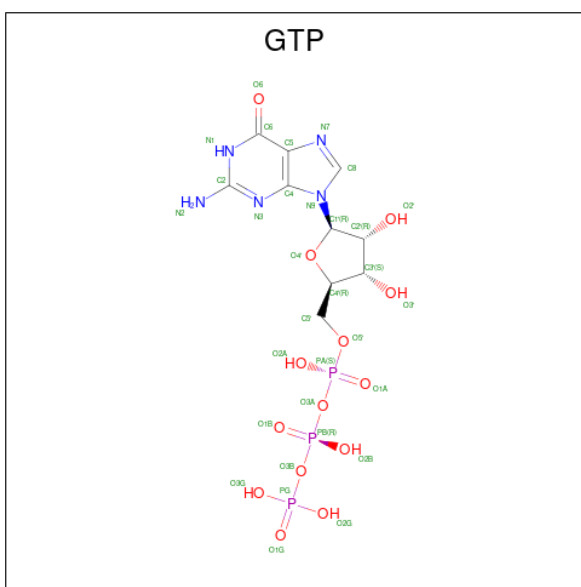
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	10	4	0
			2729	1762	457	496	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	32	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	32	0
			32	10	5	14	3		

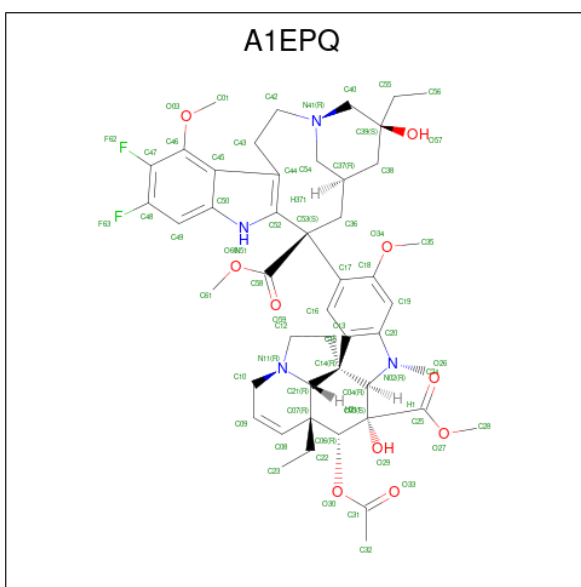
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	1	0
			1	1		
6	C	1	Total	Ca	1	0
			1	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

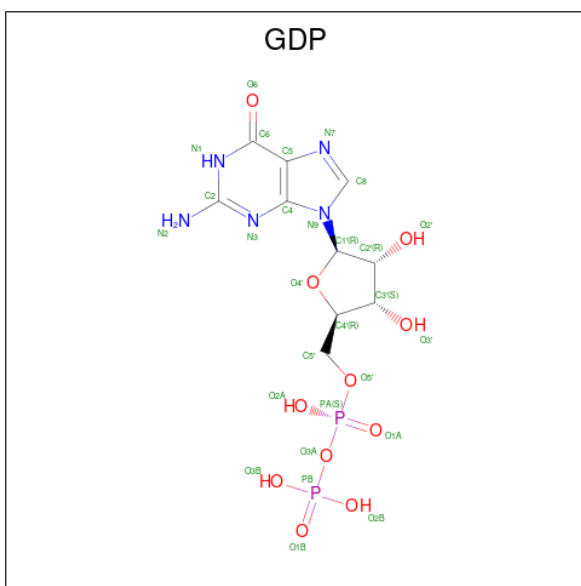
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

- Molecule 8 is 10',11'-difluoro-12'-methoxyvinblastine (CCD ID: A1EPQ) (formula: C₄₇H₅₈F₂N₄O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	F	H	N	O	0	0
			122	47	2	59	4	10		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total 28	C 10	N 5	O 11	P 2	28	0
9	B	1	Total 28	C 10	N 5	O 11	P 2	28	0

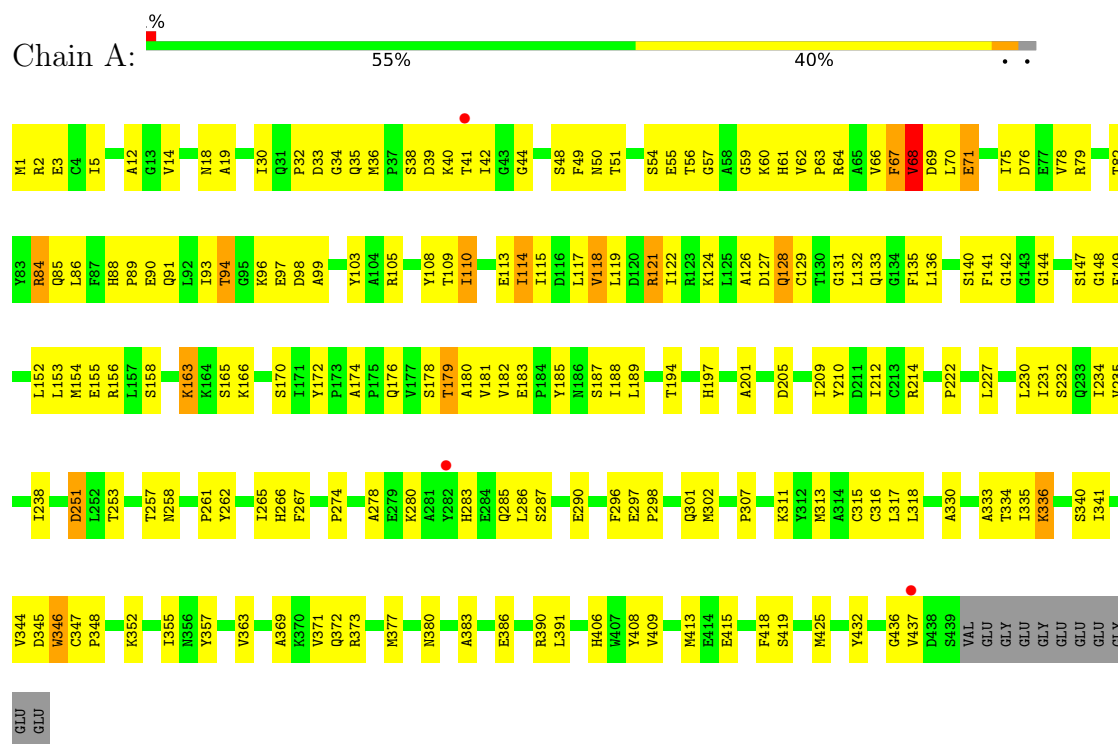
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	5	Total 5	O 5	0	0
10	B	2	Total 2	O 2	0	0

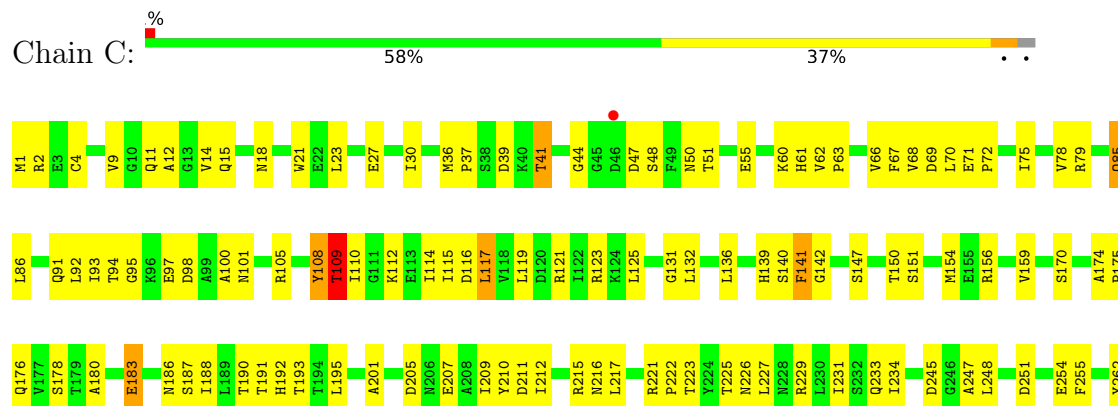
3 Residue-property plots [i](#)

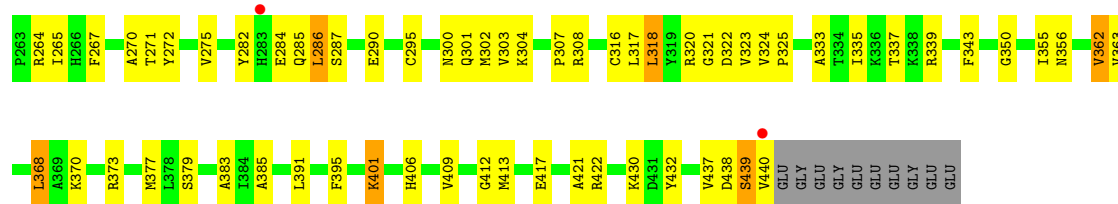
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Detyrosinated tubulin alpha-1B chain

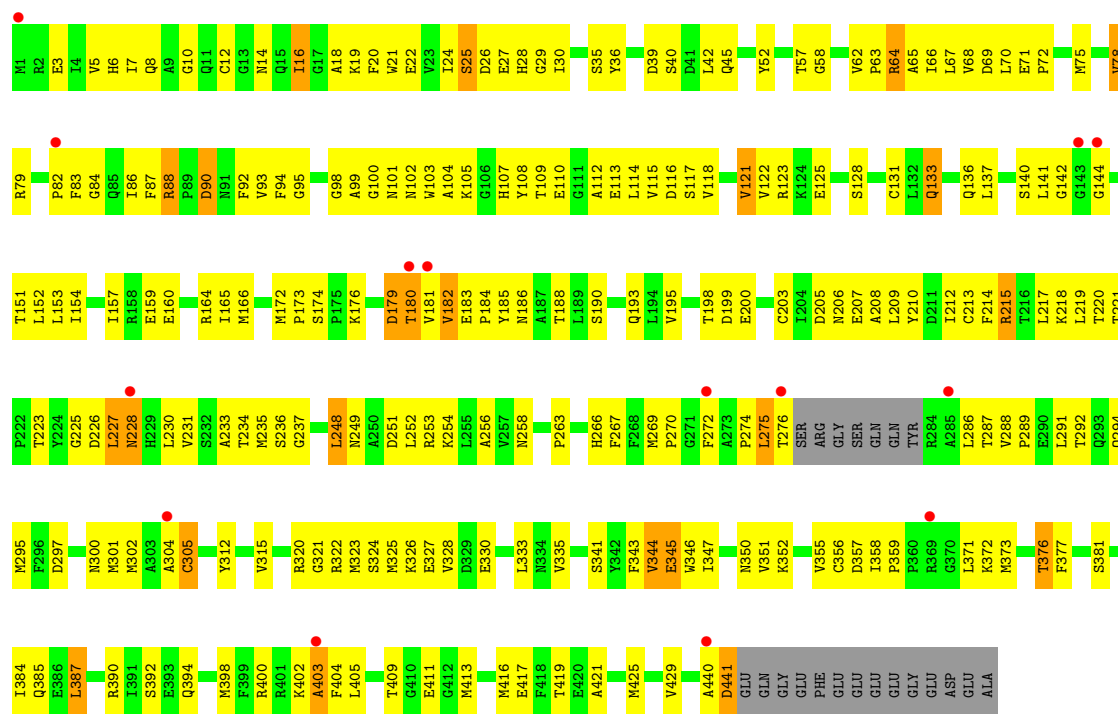
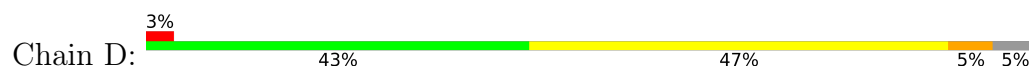


• Molecule 1: Detyrosinated tubulin alpha-1B chain

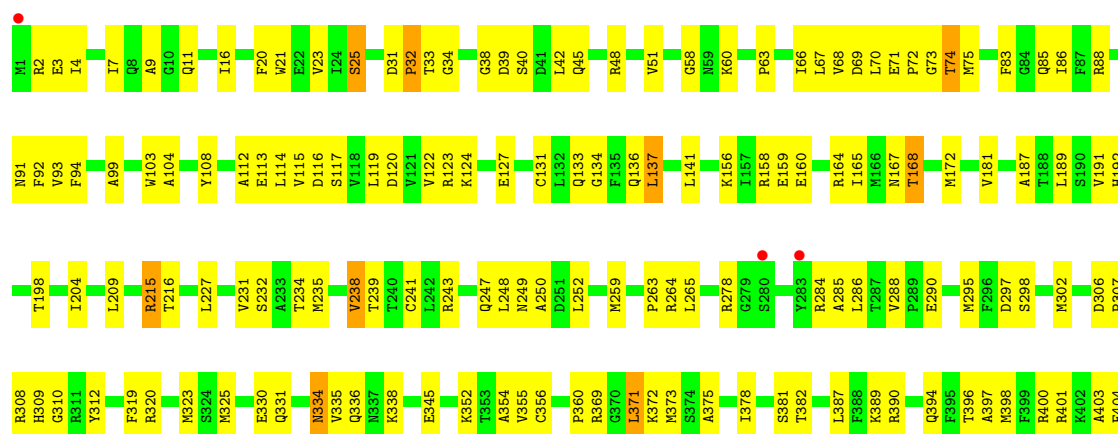


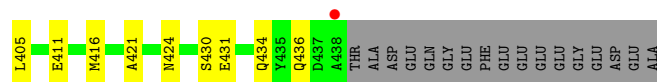


● Molecule 2: Tubulin beta-2B chain

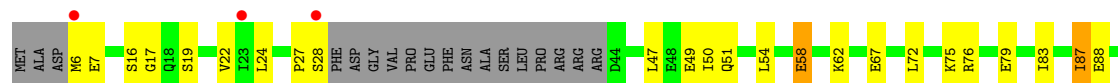


● Molecule 2: Tubulin beta-2B chain

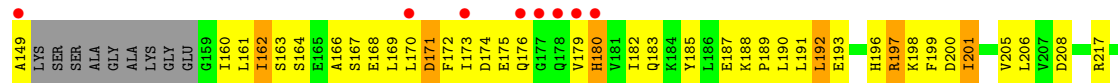
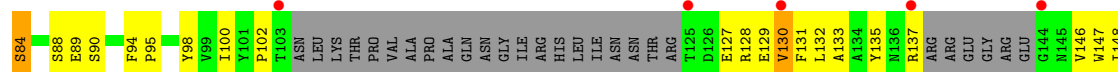
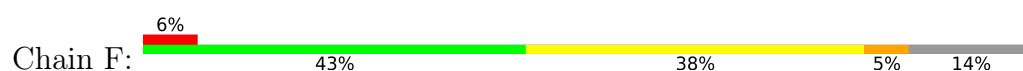




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.30Å 156.42Å 184.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.18 – 2.85 53.18 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (53.18-2.85) 99.6 (53.18-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.198 , 0.277 0.198 , 0.277	Depositor DCC
R_{free} test set	3501 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17617	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GTP, MG, GDP, A1EPQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/3571	0.58	0/4849
1	C	0.43	0/3565	0.62	0/4842
2	B	0.45	0/3451	0.61	0/4675
2	D	0.43	1/3428 (0.0%)	0.61	3/4645 (0.1%)
3	E	0.40	0/999	0.54	0/1325
4	F	0.36	0/2802	0.55	0/3789
All	All	0.42	1/17816 (0.0%)	0.59	3/24125 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	228	ASN	CG-OD1	8.42	1.39	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	228	ASN	N-CA-CB	7.20	121.88	110.73
2	D	227	LEU	CA-C-N	-5.90	113.40	122.60
2	D	227	LEU	C-N-CA	-5.90	113.40	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	41	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3465	0	3402	193	0
1	C	3466	0	3394	158	1
2	B	3370	0	3249	123	1
2	D	3343	0	3229	216	1
3	E	991	0	1012	46	0
4	F	2729	0	2715	146	1
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	C	63	59	0	4	0
9	B	28	0	12	0	0
9	D	28	0	11	0	0
10	B	2	0	0	0	0
10	C	5	0	0	0	0
All	All	17558	59	17048	851	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:504:A1EPQ:C14	8:C:504:A1EPQ:C04	1.74	1.36
2:D:75:MET:HE3	2:D:94:PHE:HB3	1.17	1.14
1:A:317:LEU:HD21	1:A:377:MET:CE	1.87	1.04
4:F:247:LYS:HE2	4:F:247:LYS:HA	1.36	1.04
2:D:75:MET:HE3	2:D:94:PHE:CB	1.90	1.01
2:D:104:ALA:HB2	2:D:413:MET:HE3	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.43	1.00
1:A:34:GLY:HA3	1:A:60:LYS:HG2	1.41	0.99
4:F:128:ARG:NH1	4:F:174:ASP:OD1	1.96	0.99
1:A:163:LYS:H	1:A:163:LYS:HE3	1.29	0.97
2:B:181:VAL:HG22	2:B:398:MET:HE1	1.45	0.95
2:D:274:PRO:HD2	2:D:371:LEU:HD13	1.47	0.95
1:A:96:LYS:H	1:A:96:LYS:HD3	1.33	0.93
2:D:93:VAL:HG21	2:D:121:VAL:HG21	1.48	0.92
2:D:402:LYS:HA	2:D:405:LEU:HD13	1.52	0.92
1:A:317:LEU:HD21	1:A:377:MET:HE2	1.50	0.90
1:C:221:ARG:HG2	2:D:325:MET:HE3	1.53	0.89
1:A:32:PRO:O	1:A:85:GLN:HG3	1.72	0.88
2:D:209:LEU:HD23	2:D:230:LEU:HD12	1.54	0.87
1:A:56:THR:HG22	1:A:60:LYS:H	1.35	0.87
1:A:234:ILE:HG12	1:A:302:MET:HE2	1.56	0.87
2:D:133:GLN:NE2	2:D:252:LEU:H	1.72	0.87
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.57	0.86
1:A:41:THR:OG1	1:A:44:GLY:O	1.94	0.86
2:D:133:GLN:HE21	2:D:252:LEU:H	1.22	0.86
1:C:142:GLY:HA3	1:C:183:GLU:HG2	1.57	0.85
3:E:50:ILE:O	3:E:54:LEU:HD12	1.77	0.85
2:D:75:MET:CE	2:D:94:PHE:HB3	2.06	0.85
2:B:264:ARG:NH1	2:B:431:GLU:OE1	2.11	0.83
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.60	0.82
1:A:56:THR:HG22	1:A:60:LYS:N	1.96	0.81
1:C:234:ILE:HD13	1:C:302:MET:HE2	1.61	0.81
1:A:88:HIS:H	1:A:91:GLN:HE21	1.28	0.80
2:D:151:THR:HB	2:D:193:GLN:HG3	1.62	0.80
2:B:345:GLU:N	2:B:345:GLU:OE1	2.15	0.80
4:F:89:GLU:N	4:F:89:GLU:OE1	2.14	0.80
2:D:16:ILE:HG22	2:D:228:ASN:HD21	1.45	0.80
1:A:119:LEU:HD11	1:A:156:ARG:CB	2.13	0.79
1:A:317:LEU:HD21	1:A:377:MET:HE3	1.63	0.79
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.63	0.79
1:C:287:SER:OG	1:C:290:GLU:HG3	1.82	0.79
3:E:83:ILE:O	3:E:87:ILE:HG13	1.83	0.79
2:D:52:TYR:OH	2:D:136:GLN:NE2	2.16	0.78
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.65	0.78
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.64	0.78
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.65	0.78
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:LEU:H	2:D:286:LEU:HD23	1.49	0.77
1:A:1:MET:HE2	1:A:50:ASN:HB3	1.67	0.77
2:B:93:VAL:HG12	2:B:114:LEU:HD11	1.67	0.77
1:A:234:ILE:O	1:A:238:ILE:HD13	1.84	0.77
2:D:114:LEU:HD12	2:D:117:SER:HB2	1.66	0.77
1:A:40:LYS:O	1:A:42:ILE:HD12	1.85	0.76
1:C:212:ILE:O	1:C:216:ASN:HB2	1.85	0.76
2:D:411:GLU:HA	3:E:137:LYS:HE3	1.68	0.76
1:C:79:ARG:HG3	1:C:92:LEU:HD12	1.68	0.76
2:D:358:ILE:HD12	2:D:358:ILE:H	1.50	0.76
1:C:221:ARG:CG	2:D:325:MET:HE3	2.16	0.75
4:F:88:SER:HG	4:F:90:SER:HG	1.31	0.75
2:B:63:PRO:HD2	2:B:86:ILE:O	1.87	0.75
1:A:262:TYR:HE1	1:A:346:TRP:CZ2	2.03	0.75
2:D:21:TRP:O	2:D:25:SER:HB2	1.85	0.75
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.69	0.75
2:D:12:CYS:CB	2:D:140:SER:HB3	2.17	0.75
2:D:104:ALA:HB2	2:D:413:MET:CE	2.14	0.75
4:F:16:GLU:O	4:F:20:LEU:HD13	1.86	0.75
1:A:234:ILE:HD12	1:A:234:ILE:H	1.50	0.74
2:B:297:ASP:HA	2:B:308:ARG:HH22	1.52	0.74
1:A:234:ILE:HG12	1:A:302:MET:CE	2.17	0.74
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.06	0.74
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.69	0.74
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.68	0.74
2:B:295:MET:CE	2:B:375:ALA:HB1	2.18	0.74
1:C:178:SER:HB2	1:C:183:GLU:OE2	1.86	0.73
1:C:209:ILE:HG22	1:C:227:LEU:HG	1.70	0.73
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.70	0.73
4:F:172:PHE:O	4:F:175:GLU:HG3	1.89	0.73
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.24	0.73
1:A:96:LYS:HD3	1:A:96:LYS:N	2.05	0.72
2:D:234:THR:HG21	2:D:270:PRO:HB2	1.71	0.72
2:B:398:MET:HE2	2:B:404:PHE:CD2	2.25	0.71
2:D:108:TYR:CD2	3:E:133:VAL:HG11	2.24	0.71
1:C:210:TYR:OH	1:C:221:ARG:HD2	1.90	0.71
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.73	0.71
2:D:12:CYS:SG	2:D:140:SER:HB3	2.31	0.71
4:F:88:SER:OG	4:F:90:SER:OG	2.09	0.71
4:F:173:ILE:HA	4:F:176:GLN:HB2	1.73	0.71
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:147:TRP:HA	4:F:185:TYR:H	1.57	0.70
3:E:75:LYS:O	3:E:79:GLU:HG3	1.91	0.70
1:C:211:ASP:OD2	1:C:304:LYS:HE3	1.92	0.69
1:C:234:ILE:CD1	1:C:302:MET:HE2	2.21	0.69
1:C:275:VAL:HG13	1:C:368:LEU:HD11	1.73	0.69
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.28	0.69
1:C:343:PHE:CE2	1:C:350:GLY:HA3	2.26	0.69
2:D:75:MET:HG3	2:D:92:PHE:HD2	1.55	0.69
2:D:112:ALA:O	2:D:115:VAL:HG12	1.92	0.69
1:A:97:GLU:OE2	2:B:164:ARG:NH2	2.25	0.69
1:C:117:LEU:HD11	1:C:121:ARG:CZ	2.23	0.69
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.75	0.69
1:A:88:HIS:N	1:A:91:GLN:HE21	1.89	0.69
2:D:301:MET:HE1	2:D:377:PHE:CD1	2.27	0.69
2:B:239:THR:O	2:B:243:ARG:HG3	1.93	0.69
2:D:93:VAL:CG2	2:D:121:VAL:HG21	2.21	0.68
1:C:188:ILE:HD11	1:C:391:LEU:HB3	1.74	0.68
2:D:102:ASN:HB3	2:D:105:LYS:HG3	1.74	0.68
2:B:398:MET:HE2	2:B:404:PHE:HD2	1.58	0.68
1:C:142:GLY:HA3	1:C:183:GLU:CG	2.23	0.68
4:F:131:PHE:CE2	4:F:170:LEU:HD21	2.28	0.68
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.75	0.68
2:B:88:ARG:O	2:B:91:ASN:HB2	1.94	0.68
2:D:10:GLY:O	2:D:14:ASN:HB2	1.93	0.68
1:A:1:MET:HE2	1:A:50:ASN:CB	2.23	0.68
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.29	0.68
2:D:217:LEU:HD11	2:D:276:THR:O	1.94	0.68
4:F:14:TYR:HA	4:F:17:VAL:HG23	1.76	0.67
2:B:20:PHE:HB2	2:B:235:MET:CE	2.25	0.67
2:D:71:GLU:HG2	2:D:98:GLY:HA2	1.77	0.67
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.30	0.67
1:C:72:PRO:HD3	1:C:95:GLY:O	1.95	0.67
2:D:16:ILE:HG13	2:D:235:MET:HE1	1.77	0.67
2:D:181:VAL:O	2:D:398:MET:HE1	1.94	0.67
1:A:88:HIS:NE2	1:A:90:GLU:HB2	2.10	0.67
1:C:156:ARG:HD3	3:E:101:LEU:CD1	2.23	0.67
4:F:78:VAL:O	4:F:82:LYS:HG3	1.95	0.66
4:F:193:GLU:OE2	4:F:196:HIS:ND1	2.28	0.66
1:A:234:ILE:HD12	1:A:234:ILE:N	2.09	0.66
4:F:274:ALA:O	4:F:276:ASN:N	2.24	0.66
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:THR:OG1	1:C:55:GLU:OE2	2.14	0.66
8:C:504:A1EPQ:C14	8:C:504:A1EPQ:C05	2.54	0.66
1:A:109:THR:O	1:A:110:ILE:HB	1.96	0.66
2:D:324:SER:O	2:D:328:VAL:HG23	1.96	0.66
2:B:334:ASN:OD1	2:B:338:LYS:HD2	1.96	0.66
2:B:58:GLY:HA3	2:B:60:LYS:NZ	2.09	0.66
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	1.78	0.65
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.78	0.65
2:D:209:LEU:CD2	2:D:230:LEU:HB2	2.26	0.65
4:F:148:ILE:HG22	4:F:183:GLN:O	1.96	0.65
2:D:400:ARG:HA	2:D:400:ARG:NE	2.11	0.65
1:C:1:MET:O	1:C:2:ARG:HB2	1.94	0.65
2:D:274:PRO:HG2	2:D:371:LEU:HD22	1.79	0.65
1:A:178:SER:HB2	1:A:183:GLU:OE2	1.96	0.65
2:D:40:SER:O	2:D:45:GLN:HG2	1.96	0.65
2:B:136:GLN:HA	2:B:167:ASN:O	1.97	0.65
4:F:243:HIS:HE1	4:F:259:GLY:O	1.79	0.65
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.32	0.65
2:B:123:ARG:O	2:B:127:GLU:HG2	1.97	0.65
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.27	0.64
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.32	0.64
1:A:311:LYS:HD2	1:A:344:VAL:HG12	1.77	0.64
1:A:180:ALA:O	1:A:183:GLU:HG3	1.96	0.64
1:C:437:VAL:HG12	1:C:438:ASP:O	1.97	0.64
2:D:321:GLY:HA2	2:D:359:PRO:HG3	1.79	0.64
3:E:125:GLU:OE1	3:E:125:GLU:HA	1.97	0.64
1:C:156:ARG:HD3	3:E:101:LEU:HD13	1.80	0.64
2:D:123:ARG:NH2	2:D:160:GLU:OE2	2.30	0.64
1:A:153:LEU:HD12	1:A:153:LEU:O	1.98	0.64
2:D:93:VAL:HG12	2:D:114:LEU:HD11	1.79	0.64
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.80	0.64
1:A:287:SER:OG	1:A:290:GLU:HG3	1.98	0.64
4:F:283:ILE:HD13	4:F:321:VAL:CG2	2.28	0.64
1:A:93:ILE:HD11	1:A:121:ARG:HG2	1.79	0.64
1:A:109:THR:O	1:A:110:ILE:CB	2.46	0.64
4:F:49:PHE:CD2	4:F:66:ARG:HD2	2.33	0.64
2:B:234:THR:O	2:B:238:VAL:HG13	1.97	0.64
2:D:223:THR:O	2:D:226:ASP:N	2.30	0.63
2:D:275:LEU:HG	2:D:300:ASN:ND2	2.13	0.63
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.79	0.63
4:F:81:ILE:HD12	4:F:94:PHE:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:278:THR:HG22	4:F:280:GLU:H	1.62	0.63
1:A:155:GLU:HG2	1:A:197:HIS:NE2	2.14	0.63
4:F:22:LEU:O	4:F:24:THR:N	2.31	0.63
1:C:211:ASP:HB3	1:C:215:ARG:NH1	2.13	0.63
4:F:147:TRP:CB	4:F:182:ILE:HD11	2.29	0.63
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.34	0.63
2:B:23:VAL:HG21	2:B:232:SER:OG	1.99	0.63
1:C:23:LEU:O	1:C:27:GLU:HG3	1.98	0.63
2:D:29:GLY:O	2:D:36:TYR:HA	1.98	0.63
2:D:215:ARG:O	2:D:218:LYS:HD2	1.99	0.63
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.13	0.62
4:F:34:ASN:HD22	4:F:35:PRO:HD2	1.63	0.62
2:D:274:PRO:HG3	2:D:286:LEU:HD21	1.81	0.62
2:D:416:MET:HA	2:D:419:THR:OG1	1.99	0.62
2:B:331:GLN:O	2:B:335:VAL:HG23	1.98	0.62
2:D:16:ILE:CG2	2:D:228:ASN:HD21	2.11	0.62
2:D:90:ASP:OD1	2:D:90:ASP:N	2.26	0.62
1:A:96:LYS:NZ	1:A:113:GLU:OE2	2.27	0.62
1:C:439:SER:HB3	2:B:401:ARG:HD3	1.81	0.62
2:D:288:VAL:HB	2:D:327:GLU:OE2	1.99	0.62
4:F:31:ARG:HD3	4:F:32:LYS:H	1.65	0.62
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.35	0.62
4:F:228:TYR:HA	4:F:238:CYS:HB2	1.80	0.61
1:A:19:ALA:HB1	1:A:232:SER:OG	2.00	0.61
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.82	0.61
4:F:348:GLN:HG3	4:F:352:ASP:OD2	2.00	0.61
1:A:355:ILE:O	3:E:17:GLY:HA3	1.99	0.61
1:C:41:THR:OG1	1:C:41:THR:O	2.18	0.61
2:B:295:MET:HE3	2:B:375:ALA:HB1	1.81	0.61
1:C:406:HIS:ND1	2:D:263:PRO:HG3	2.16	0.61
2:D:326:LYS:HE2	2:D:330:GLU:OE2	2.00	0.61
4:F:31:ARG:HD3	4:F:32:LYS:N	2.16	0.61
4:F:131:PHE:CE1	4:F:182:ILE:HG12	2.35	0.61
2:D:174:SER:HB2	2:D:207:GLU:N	2.16	0.61
4:F:80:LEU:O	4:F:84:SER:OG	2.13	0.61
1:A:227:LEU:O	1:A:231:ILE:HG13	2.00	0.61
1:C:215:ARG:HG3	1:C:215:ARG:HH11	1.64	0.61
2:D:200:GLU:OE1	2:D:256:ALA:HB2	2.01	0.60
1:A:285:GLN:HG3	1:A:372[B]:GLN:NE2	2.16	0.60
1:C:265:ILE:HG23	1:C:432:TYR:CE1	2.37	0.60
2:D:16:ILE:HG22	2:D:228:ASN:ND2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:HH11	2:B:124:LYS:HE3	1.65	0.60
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.01	0.60
2:D:179:ASP:OD1	2:D:179:ASP:N	2.35	0.60
1:A:141:PHE:O	1:A:147:SER:HB3	2.01	0.60
4:F:237:THR:HG23	4:F:249:TYR:CD2	2.36	0.60
4:F:31:ARG:HD2	4:F:32:LYS:HG2	1.84	0.60
2:B:416:MET:HA	2:B:416:MET:HE2	1.82	0.60
4:F:283:ILE:HD13	4:F:321:VAL:HG21	1.83	0.60
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.84	0.60
1:A:56:THR:CG2	1:A:60:LYS:H	2.11	0.60
4:F:131:PHE:HE2	4:F:170:LEU:HD21	1.67	0.60
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.84	0.59
2:D:101:ASN:ND2	2:D:180:THR:HG21	2.16	0.59
2:D:221:THR:HG23	2:D:221:THR:O	2.02	0.59
4:F:162:ILE:HG13	4:F:236:LYS:HE2	1.85	0.59
4:F:237:THR:HG23	4:F:249:TYR:CE2	2.37	0.59
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.85	0.59
1:A:408:TYR:CD2	1:A:418:PHE:HZ	2.20	0.59
1:C:18:ASN:HD21	1:C:78:VAL:CG2	2.15	0.59
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.32	0.59
4:F:40:MET:CE	4:F:47:LEU:HG	2.32	0.59
1:A:234:ILE:CG1	1:A:302:MET:HE2	2.32	0.59
2:D:102:ASN:HB3	2:D:105:LYS:CG	2.33	0.59
2:B:20:PHE:HB2	2:B:235:MET:HE3	1.84	0.59
4:F:40:MET:HE3	4:F:42:GLY:HA2	1.83	0.59
4:F:98:TYR:HB3	4:F:127:GLU:HB2	1.85	0.59
4:F:55:GLU:HB3	4:F:58:LEU:HD12	1.85	0.58
4:F:65:TYR:OH	4:F:208:ASP:O	2.21	0.58
2:B:67:LEU:N	2:B:67:LEU:HD12	2.18	0.58
2:B:284:ARG:NH1	2:B:285:ALA:O	2.36	0.58
1:C:333:ALA:O	1:C:337:THR:HG23	2.03	0.58
2:D:118:VAL:O	2:D:121:VAL:HG23	2.02	0.58
2:D:209:LEU:HD23	2:D:230:LEU:CD1	2.31	0.58
2:B:32:PRO:O	2:B:85:GLN:HG3	2.03	0.58
4:F:162:ILE:H	4:F:236:LYS:HE2	1.67	0.58
1:C:192:HIS:CG	1:C:421:ALA:HA	2.38	0.58
1:A:3:GLU:HG2	1:A:64:ARG:NE	2.17	0.58
2:D:231:VAL:CG1	2:D:235:MET:HE3	2.33	0.58
4:F:171:ASP:OD1	4:F:171:ASP:N	2.34	0.58
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.38	0.58
2:D:42:LEU:HD22	2:D:42:LEU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ILE:HG23	4:F:128:ARG:HD3	1.85	0.58
1:A:105:ARG:O	1:A:109:THR:O	2.21	0.58
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.03	0.58
1:C:70:LEU:HD13	1:C:110:ILE:HG22	1.86	0.58
2:D:27:GLU:OE2	2:D:236:SER:OG	2.17	0.58
2:D:220:THR:O	2:D:221:THR:HG22	2.04	0.58
4:F:149:ALA:HB3	4:F:160:ILE:HG23	1.86	0.58
2:B:123:ARG:NH1	2:B:160:GLU:OE2	2.36	0.58
4:F:100:ILE:HG23	4:F:128:ARG:CD	2.34	0.57
4:F:277[A]:THR:OG1	4:F:278:THR:N	2.37	0.57
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.38	0.57
1:A:96:LYS:HG2	1:A:97:GLU:H	1.69	0.57
3:E:72:LEU:HD11	2:B:158:ARG:HG2	1.86	0.57
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.04	0.57
2:B:323:MET:HE2	2:B:373:MET:SD	2.45	0.57
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.32	0.57
1:A:163:LYS:HE3	1:A:163:LYS:N	2.11	0.57
1:C:109:THR:HG22	1:C:110:ILE:N	2.19	0.57
2:D:320:ARG:HA	2:D:356:CYS:O	2.05	0.57
2:D:387:LEU:HD23	2:D:387:LEU:C	2.30	0.57
3:E:47:LEU:HD12	3:E:47:LEU:O	2.03	0.57
1:A:33:ASP:O	1:A:60:LYS:HG3	2.05	0.57
2:D:274:PRO:CD	2:D:371:LEU:HD13	2.29	0.57
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.34	0.57
1:A:66[A]:VAL:HG23	1:A:91:GLN:O	2.05	0.57
1:A:113:GLU:O	1:A:113:GLU:HG2	2.05	0.57
4:F:22:LEU:C	4:F:24:THR:H	2.12	0.57
2:B:141:LEU:HD12	2:B:172:MET:SD	2.44	0.57
3:E:140:LYS:C	3:E:140:LYS:HD2	2.29	0.57
2:D:234:THR:CG2	2:D:270:PRO:HB2	2.35	0.56
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.87	0.56
2:B:286:LEU:HD12	2:B:290:GLU:HB3	1.86	0.56
1:A:158:SER:OG	1:A:166:LYS:NZ	2.37	0.56
1:A:163:LYS:H	1:A:163:LYS:CE	2.13	0.56
1:A:201:ALA:HB3	1:A:267:PHE:CD2	2.41	0.56
1:C:209:ILE:CG2	1:C:227:LEU:HG	2.36	0.56
3:E:51:GLN:OE1	3:E:51:GLN:HA	2.04	0.56
2:D:42:LEU:HD22	2:D:42:LEU:N	2.21	0.56
2:B:298:SER:OG	2:B:308:ARG:NH1	2.39	0.56
1:A:141:PHE:HB3	1:A:187:SER:OG	2.06	0.56
1:C:413:MET:HA	1:C:417[B]:GLU:OE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:OG1	1:A:41:THR:O	2.24	0.56
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.41	0.56
1:A:280:LYS:HE2	1:A:283:HIS:ND1	2.20	0.56
2:D:209:LEU:HD22	2:D:227:LEU:O	2.05	0.56
2:B:104:ALA:O	2:B:108:TYR:HB2	2.06	0.56
2:D:159:GLU:HG3	3:E:123:LEU:HB3	1.87	0.56
1:A:231:ILE:O	1:A:235:VAL:HG23	2.06	0.56
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.41	0.55
1:C:271:THR:HG21	1:C:295:CYS:O	2.06	0.55
4:F:247:LYS:HE2	4:F:247:LYS:CA	2.24	0.55
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.88	0.55
1:C:248:LEU:N	1:C:248:LEU:HD23	2.22	0.55
1:C:323:VAL:HG12	1:C:355:ILE:HD13	1.88	0.55
2:D:294:GLN:O	2:D:297:ASP:HB3	2.05	0.55
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.89	0.55
2:D:223:THR:O	2:D:226:ASP:HB2	2.06	0.55
2:B:11:GLN:HA	2:B:74:THR:HG21	1.88	0.55
1:A:286:LEU:O	1:A:373:ARG:NH1	2.40	0.55
3:E:135:LYS:O	3:E:139:LEU:HG	2.06	0.55
4:F:130:VAL:O	4:F:133:ALA:HB3	2.05	0.55
4:F:292:ARG:HD2	4:F:380:HIS:HB3	1.87	0.55
4:F:167:SER:C	4:F:169:LEU:H	2.14	0.55
1:C:101:ASN:OD1	2:D:254:LYS:HD3	2.07	0.55
1:C:91:GLN:C	1:C:92:LEU:HD23	2.31	0.55
4:F:102:PRO:HA	4:F:174:ASP:HA	1.88	0.55
4:F:168:GLU:N	4:F:171:ASP:OD1	2.40	0.55
1:A:56:THR:O	1:A:59:GLY:N	2.24	0.55
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.41	0.55
1:C:227:LEU:O	1:C:231:ILE:HG13	2.07	0.55
2:D:166:MET:HG3	2:D:198:THR:HG22	1.88	0.55
2:D:184:PRO:HG3	2:D:394:GLN:HB3	1.87	0.55
2:D:203:CYS:SG	2:D:267:PHE:HB3	2.47	0.55
1:A:262:TYR:CE1	1:A:346:TRP:CH2	2.94	0.54
1:A:413:MET:HE1	1:A:418:PHE:CE2	2.43	0.54
2:D:93:VAL:HG21	2:D:121:VAL:CG2	2.30	0.54
3:E:106:GLU:HA	3:E:106:GLU:OE1	2.06	0.54
4:F:200:ASP:OD2	4:F:222:ARG:HG3	2.07	0.54
4:F:32:LYS:HG3	4:F:33:ASP:N	2.22	0.54
2:B:48:ARG:O	2:B:51:VAL:HG23	2.07	0.54
1:A:230:LEU:O	1:A:234:ILE:HD13	2.07	0.54
2:D:288:VAL:HG11	2:D:327:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PRO:HG2	2:B:371:LEU:HB2	1.90	0.54
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.72	0.54
2:D:66:ILE:HD13	2:D:122:VAL:HG22	1.89	0.54
4:F:237:THR:O	4:F:246:GLN:NE2	2.40	0.54
2:D:14:ASN:ND2	2:D:68:VAL:O	2.41	0.54
1:C:440:VAL:HG22	1:C:440:VAL:O	2.07	0.54
4:F:135:TYR:OH	4:F:164:SER:O	2.23	0.54
4:F:189:PRO:O	4:F:191:LEU:HG	2.07	0.54
2:B:32:PRO:O	2:B:86:ILE:HG23	2.08	0.54
2:B:7:ILE:O	2:B:137:LEU:HA	2.08	0.54
1:A:212:ILE:HG21	1:A:230:LEU:HD21	1.89	0.54
1:C:156:ARG:CD	3:E:101:LEU:CD1	2.86	0.54
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.08	0.54
1:C:335:ILE:HG13	1:C:339:ARG:HD2	1.89	0.54
2:D:248:LEU:HD11	2:D:352:LYS:CB	2.37	0.54
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.36	0.54
2:D:292:THR:HG22	2:D:335:VAL:CG2	2.37	0.53
1:A:234:ILE:H	1:A:234:ILE:CD1	2.17	0.53
1:C:362:VAL:HG22	1:C:370:LYS:HG3	1.91	0.53
1:C:395:PHE:CD1	1:C:422:ARG:HD3	2.43	0.53
4:F:199:PHE:CG	4:F:221:LEU:HD23	2.43	0.53
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.08	0.53
1:C:271:THR:CG2	1:C:295:CYS:HA	2.38	0.53
1:C:156:ARG:CD	3:E:101:LEU:HD11	2.39	0.53
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.90	0.53
1:C:60:LYS:HG2	1:C:62:VAL:HG22	1.90	0.53
1:C:100:ALA:HB2	2:D:253:ARG:HD2	1.90	0.53
2:D:66:ILE:HD11	2:D:122:VAL:HA	1.90	0.53
2:B:16:ILE:O	2:B:235:MET:HE1	2.07	0.53
1:A:238:ILE:HD12	1:A:238:ILE:N	2.24	0.53
2:B:58:GLY:HA3	2:B:60:LYS:HZ3	1.72	0.53
4:F:14:TYR:CD1	4:F:17:VAL:HG21	2.42	0.53
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.39	0.53
1:C:66:VAL:CG1	1:C:68[A]:VAL:HG23	2.39	0.53
2:D:205:ASP:OD1	2:D:390:ARG:NH2	2.42	0.53
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.44	0.53
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.43	0.53
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.74	0.53
1:A:109:THR:O	1:A:110:ILE:HG13	2.08	0.52
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.21	0.52
2:D:205:ASP:CG	2:D:390:ARG:HH22	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:55:GLU:CB	4:F:58:LEU:HD12	2.40	0.52
2:B:40:SER:OG	2:B:42:LEU:HB2	2.09	0.52
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.92	0.52
1:A:297:GLU:HA	1:A:297:GLU:OE1	2.08	0.52
1:C:151[A]:SER:HB2	1:C:193:THR:HG22	1.91	0.52
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.44	0.52
4:F:173:ILE:HD12	4:F:180:HIS:HB2	1.91	0.52
2:B:31:ASP:O	2:B:33:THR:N	2.42	0.52
1:A:386:GLU:O	1:A:390:ARG:HG2	2.10	0.52
2:D:98:GLY:O	2:D:100:GLY:N	2.37	0.52
2:D:172:MET:HE3	2:D:173:PRO:HD2	1.92	0.52
1:A:3:GLU:HB3	1:A:64:ARG:CD	2.40	0.52
1:A:88:HIS:HB3	1:A:91:GLN:HG2	1.92	0.52
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.92	0.52
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.44	0.52
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.09	0.52
3:E:6:MET:O	3:E:6:MET:HG2	2.10	0.52
4:F:132:LEU:O	4:F:135:TYR:N	2.42	0.52
2:B:69:ASP:O	2:B:94:PHE:HA	2.10	0.52
2:B:119:LEU:HD11	2:B:156:LYS:HD3	1.92	0.52
1:A:34:GLY:HA3	1:A:60:LYS:CG	2.27	0.52
1:C:69:ASP:O	1:C:94:THR:HA	2.10	0.52
1:C:210:TYR:HH	1:C:221:ARG:HD2	1.75	0.52
1:C:234:ILE:HD13	1:C:302:MET:CE	2.36	0.52
2:D:114:LEU:O	2:D:117:SER:N	2.43	0.52
2:B:382:THR:OG1	2:B:436:GLN:HG3	2.09	0.52
1:A:119:LEU:HD11	1:A:156:ARG:CG	2.39	0.52
1:C:223:THR:O	1:C:227:LEU:HD13	2.10	0.52
2:B:31:ASP:C	2:B:33:THR:H	2.17	0.51
2:B:264:ARG:NH2	2:B:424:ASN:OD1	2.43	0.51
1:A:296:PHE:CE2	1:A:341:ILE:HD13	2.45	0.51
4:F:100:ILE:CD1	4:F:128:ARG:HG2	2.39	0.51
2:D:269:MET:CE	2:D:301:MET:SD	2.99	0.51
2:B:231:VAL:O	2:B:235:MET:HG3	2.10	0.51
2:B:372:LYS:C	2:B:373:MET:HG2	2.36	0.51
1:C:48:SER:O	1:C:51:THR:HG23	2.10	0.51
2:D:343:PHE:CE2	2:D:351:VAL:HG21	2.46	0.51
4:F:137:ARG:C	4:F:137:ARG:HE	2.18	0.51
4:F:243:HIS:CE1	4:F:259:GLY:O	2.62	0.51
1:C:11:GLN:O	1:C:15:GLN:HG3	2.11	0.51
1:C:217:LEU:HD11	1:C:368:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:LEU:HD21	2:D:87:PHE:CE2	2.45	0.51
2:D:93:VAL:CG1	2:D:114:LEU:HD11	2.41	0.51
3:E:72:LEU:HD13	2:B:159:GLU:HB2	1.93	0.51
2:B:75:MET:SD	2:B:94:PHE:HB3	2.50	0.51
1:A:99:ALA:HB3	1:A:144:GLY:HA3	1.92	0.51
1:A:335:ILE:C	1:A:335:ILE:HD12	2.36	0.51
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.51
4:F:4:PHE:HD1	4:F:27:TRP:HE3	1.59	0.51
2:B:9:ALA:HA	2:B:68:VAL:O	2.11	0.51
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.93	0.51
2:D:114:LEU:HD12	2:D:117:SER:CB	2.40	0.51
2:D:237:GLY:HA3	2:D:376:THR:CG2	2.36	0.51
2:B:372:LYS:O	2:B:373:MET:HG2	2.11	0.51
4:F:173:ILE:HD11	4:F:180:HIS:H	1.75	0.51
2:B:115:VAL:HG13	2:B:116:ASP:N	2.26	0.51
2:B:187:ALA:O	2:B:191:VAL:HG23	2.11	0.51
2:B:390:ARG:O	2:B:394:GLN:HG3	2.11	0.51
2:D:18:ALA:O	2:D:22:GLU:HG3	2.11	0.50
1:C:210:TYR:CE1	1:C:222:PRO:HG2	2.47	0.50
1:A:48:SER:O	1:A:51[A]:THR:HG23	2.11	0.50
4:F:283:ILE:CD1	4:F:321:VAL:HG21	2.42	0.50
2:B:3:GLU:O	2:B:133:GLN:HG2	2.11	0.50
1:A:174:ALA:O	1:A:178:SER:HB3	2.12	0.50
1:C:221:ARG:HG2	2:D:325:MET:CE	2.32	0.50
4:F:7:ARG:NE	4:F:43:GLU:OE1	2.38	0.50
4:F:100:ILE:HD12	4:F:128:ARG:HG2	1.92	0.50
1:A:63:PRO:CG	1:A:86:LEU:HD21	2.41	0.50
1:A:108:TYR:HE2	1:A:413:MET:HG3	1.75	0.50
2:D:69:ASP:N	2:D:75:MET:HE1	2.26	0.50
4:F:129:GLU:OE1	4:F:129:GLU:HA	2.11	0.50
3:E:58:GLU:O	3:E:62:LYS:HG3	2.12	0.50
1:A:36:MET:HE1	1:A:49:PHE:CE2	2.47	0.50
1:A:127:ASP:C	1:A:129:CYS:H	2.20	0.50
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.42	0.50
1:A:317:LEU:CD2	1:A:377:MET:HE3	2.37	0.50
2:D:63:PRO:O	2:D:65:ALA:N	2.43	0.50
3:E:6:MET:N	3:E:24:LEU:HD23	2.27	0.50
2:B:75:MET:HG3	2:B:94:PHE:CG	2.47	0.50
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.94	0.49
1:A:66[B]:VAL:HG23	1:A:91:GLN:O	2.12	0.49
1:A:437:VAL:HG12	1:A:437:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:274:PRO:HG3	2:D:286:LEU:CD2	2.42	0.49
4:F:20:LEU:HD23	4:F:348:GLN:OE1	2.12	0.49
4:F:361:LEU:O	4:F:362:ALA:HB2	2.11	0.49
2:B:34:GLY:O	2:B:60:LYS:HA	2.11	0.49
1:A:114:ILE:HG12	1:A:114:ILE:O	2.12	0.49
1:C:301:GLN:OE1	1:C:307:PRO:HG3	2.12	0.49
2:D:115:VAL:HG13	2:D:116:ASP:N	2.27	0.49
2:D:193:GLN:OE1	3:E:126:LYS:HE2	2.12	0.49
1:A:317:LEU:CD2	1:A:377:MET:HE2	2.33	0.49
1:C:123:ARG:O	1:C:123:ARG:HD3	2.12	0.49
1:C:286:LEU:O	1:C:373:ARG:NH1	2.43	0.49
1:C:141:PHE:O	1:C:147:SER:HB3	2.11	0.49
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.42	0.49
1:C:412:GLY:HA3	3:E:108:ASN:ND2	2.27	0.49
2:B:192:HIS:CG	2:B:421:ALA:HA	2.48	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.95	0.49
1:C:175:PRO:HD2	1:C:176:GLN:OE1	2.12	0.49
2:D:101:ASN:HA	2:D:144:GLY:HA2	1.94	0.49
2:D:403:ALA:HB1	2:D:404:PHE:CD2	2.46	0.49
4:F:30:LEU:HD13	4:F:34:ASN:OD1	2.12	0.49
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.53	0.49
1:A:88:HIS:ND1	1:A:89:PRO:HD2	2.28	0.49
1:A:103:TYR:HD2	1:A:189:LEU:HD13	1.74	0.49
2:B:416:MET:HA	2:B:416:MET:CE	2.40	0.49
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.43	0.49
4:F:161:LEU:HD23	4:F:169:LEU:HA	1.93	0.49
2:B:58:GLY:HA3	2:B:60:LYS:HZ2	1.76	0.49
2:B:71:GLU:HG3	2:B:72:PRO:HD2	1.93	0.49
1:C:225:THR:O	1:C:229:ARG:HD3	2.12	0.49
1:C:323:VAL:HG12	1:C:355:ILE:CD1	2.42	0.49
2:D:186:ASN:O	2:D:190:SER:HB2	2.13	0.49
2:D:325:MET:SD	2:D:355:VAL:HG21	2.53	0.49
2:B:83:PHE:HD2	2:B:86:ILE:HD13	1.76	0.49
1:A:44:GLY:O	1:A:55:GLU:OE2	2.31	0.49
2:D:231:VAL:HG12	2:D:235:MET:HE3	1.94	0.49
3:E:136:ASN:OD1	3:E:139:LEU:HD12	2.12	0.49
4:F:200:ASP:O	4:F:221:LEU:HA	2.13	0.49
1:C:186:ASN:O	1:C:190:THR:HG22	2.13	0.49
1:C:217:LEU:HD11	1:C:368:LEU:CD1	2.42	0.48
4:F:34:ASN:ND2	4:F:35:PRO:HD2	2.28	0.48
4:F:217:ARG:HG2	4:F:374:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.94	0.48
1:A:118:VAL:HG11	1:A:153:LEU:HD22	1.95	0.48
1:A:298:PRO:HA	1:A:301:GLN:CD	2.38	0.48
2:D:322:ARG:NH1	2:D:357:ASP:OD1	2.46	0.48
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.96	0.48
2:D:104:ALA:CB	2:D:413:MET:HE3	2.27	0.48
2:D:172:MET:HB2	2:D:205:ASP:HA	1.95	0.48
2:D:345:GLU:OE2	2:D:440:ALA:N	2.46	0.48
3:E:76:ARG:NE	2:B:159:GLU:OE1	2.36	0.48
1:A:234:ILE:O	1:A:238:ILE:CD1	2.59	0.48
3:E:123:LEU:N	3:E:123:LEU:HD23	2.29	0.48
2:B:234:THR:OG1	2:B:302:MET:HE3	2.13	0.48
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.48
4:F:2:TYR:HB2	4:F:27:TRP:CE2	2.49	0.48
2:B:248:LEU:CD1	2:B:352:LYS:HB3	2.44	0.48
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.66	0.48
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.49	0.48
2:D:39:ASP:OD1	2:D:40:SER:N	2.43	0.48
2:B:387:LEU:C	2:B:387:LEU:HD12	2.39	0.48
1:A:179:THR:HG21	2:B:247:GLN:HB3	1.95	0.48
1:A:88:HIS:H	1:A:91:GLN:NE2	2.06	0.47
1:C:318:LEU:N	1:C:318:LEU:CD1	2.77	0.47
2:D:72:PRO:HB3	2:D:94:PHE:CD1	2.49	0.47
4:F:173:ILE:HD12	4:F:180:HIS:CB	2.44	0.47
4:F:299:GLU:N	4:F:300:PRO:HD2	2.28	0.47
1:C:195:LEU:HD23	1:C:264:ARG:NH1	2.29	0.47
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.96	0.47
2:D:312:TYR:CD1	2:D:381:SER:HB2	2.49	0.47
4:F:271:LEU:O	4:F:274:ALA:O	2.32	0.47
1:A:36:MET:HE1	1:A:49:PHE:CZ	2.49	0.47
1:A:409:VAL:HA	1:A:413:MET:O	2.14	0.47
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.15	0.47
2:D:83:PHE:O	2:D:86:ILE:HG22	2.14	0.47
3:E:136:ASN:O	3:E:139:LEU:HB2	2.14	0.47
2:B:387:LEU:HD12	2:B:387:LEU:O	2.14	0.47
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.14	0.47
4:F:205:VAL:HG11	4:F:291:ILE:HG21	1.96	0.47
1:A:413:MET:HE1	1:A:418:PHE:CD2	2.50	0.47
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.42	0.47
1:C:108:TYR:HD2	3:E:105:MET:SD	2.37	0.47
2:D:28:HIS:HA	2:D:45:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:MET:HE2	4:F:3:THR:HG23	1.96	0.47
4:F:256:TYR:HB2	4:F:257:GLU:OE2	2.14	0.47
2:B:71:GLU:HG2	2:B:73:GLY:H	1.79	0.47
2:B:88:ARG:NH1	2:B:124:LYS:HE3	2.30	0.47
1:A:67:PHE:CD1	1:A:67:PHE:N	2.83	0.47
2:D:286:LEU:CD1	2:D:294:GLN:OE1	2.63	0.47
2:D:322:ARG:HD2	2:D:322:ARG:HA	1.74	0.47
4:F:201:ILE:HB	4:F:319:PHE:HB2	1.97	0.47
1:C:41:THR:HB	1:C:44:GLY:O	2.15	0.47
2:D:69:ASP:CB	2:D:75:MET:HE1	2.44	0.47
1:A:93:ILE:HD11	1:A:121:ARG:CG	2.45	0.47
1:C:192:HIS:CD2	1:C:421:ALA:HA	2.50	0.47
1:C:251:ASP:HB2	1:C:254:GLU:HG3	1.96	0.47
1:C:262:TYR:HB2	1:C:265:ILE:HD12	1.97	0.47
4:F:292:ARG:HG3	4:F:378:LEU:HB3	1.96	0.47
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.98	0.46
1:A:39:ASP:OD2	1:A:41:THR:OG1	2.33	0.46
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.50	0.46
1:C:285:GLN:HG3	1:C:373:ARG:HH12	1.80	0.46
2:D:7:ILE:O	2:D:137:LEU:HD12	2.16	0.46
2:D:441:ASP:N	2:D:441:ASP:OD1	2.49	0.46
1:A:317:LEU:CD2	1:A:377:MET:CE	2.77	0.46
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.79	0.46
1:C:47:ASP:O	1:C:50:ASN:HB2	2.16	0.46
1:C:174:ALA:HB2	1:C:207:GLU:N	2.30	0.46
2:D:234:THR:OG1	2:D:302:MET:HE3	2.15	0.46
4:F:225:SER:OG	4:F:250:SER:HA	2.15	0.46
1:A:79:ARG:HH12	1:A:94:THR:CG2	2.28	0.46
1:A:88:HIS:HB3	1:A:91:GLN:CG	2.46	0.46
1:C:308:ARG:HB2	1:C:308:ARG:NH1	2.30	0.46
2:D:153:LEU:O	2:D:157:ILE:HG13	2.16	0.46
2:D:208:ALA:O	2:D:212:ILE:HG12	2.15	0.46
2:D:210:TYR:O	2:D:213:CYS:N	2.49	0.46
4:F:47:LEU:C	4:F:47:LEU:HD23	2.40	0.46
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.15	0.46
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.96	0.46
1:C:41:THR:O	1:C:55:GLU:OE1	2.34	0.46
1:C:60:LYS:NZ	1:C:85:GLN:O	2.29	0.46
1:C:321:GLY:O	1:C:323:VAL:N	2.49	0.46
2:D:292:THR:CG2	2:D:335:VAL:CG2	2.94	0.46
2:D:321:GLY:O	2:D:323:MET:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LEU:HD11	2:B:352:LYS:HB3	1.96	0.46
1:A:155:GLU:HA	1:A:197:HIS:CD2	2.50	0.46
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.55	0.46
1:C:115:ILE:HG23	1:C:116:ASP:N	2.30	0.46
1:C:409:VAL:HA	1:C:413:MET:O	2.16	0.46
2:D:141:LEU:HD12	2:D:172:MET:SD	2.56	0.46
4:F:200:ASP:HB3	4:F:222:ARG:HB2	1.98	0.46
1:A:88:HIS:HB3	1:A:91:GLN:CD	2.41	0.46
1:C:222:PRO:HA	1:C:226:ASN:OD1	2.16	0.46
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.98	0.46
2:D:392:SER:HB2	2:D:425:MET:HE3	1.98	0.46
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.49	0.46
1:A:313:MET:HE3	1:A:380:ASN:OD1	2.15	0.46
1:A:345:ASP:C	1:A:347:CYS:H	2.24	0.46
1:C:212:ILE:HD11	1:C:300:ASN:HA	1.97	0.46
2:B:4:ILE:HD13	2:B:252:LEU:HD11	1.96	0.46
3:E:76:ARG:NH1	3:E:79:GLU:OE2	2.49	0.46
4:F:147:TRP:HB3	4:F:182:ILE:CD1	2.46	0.46
2:B:21:TRP:O	2:B:25:SER:HB2	2.15	0.46
2:B:397:ALA:HA	2:B:400:ARG:NH1	2.31	0.46
1:A:330:ALA:O	1:A:333:ALA:HB3	2.16	0.45
1:C:150:THR:O	1:C:154:MET:HG2	2.16	0.45
1:C:215:ARG:NH1	1:C:215:ARG:HG3	2.31	0.45
4:F:338:CYS:O	4:F:343:TYR:CE2	2.69	0.45
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.98	0.45
4:F:278:THR:O	4:F:282:SER:OG	2.28	0.45
2:B:134:GLY:HA3	2:B:165:ILE:O	2.16	0.45
2:D:30:ILE:HA	2:D:35:SER:O	2.16	0.45
2:D:137:LEU:HD23	2:D:154:ILE:HD11	1.99	0.45
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.98	0.45
2:B:238:VAL:HB	2:B:378:ILE:HD11	1.99	0.45
2:B:319:PHE:HB2	2:B:355:VAL:HG22	1.99	0.45
1:A:69:ASP:N	1:A:75:ILE:HD11	2.32	0.45
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.40	0.45
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.10	0.45
2:D:287:THR:HB	2:D:289:PRO:HD2	1.98	0.45
1:A:154:MET:HG3	1:A:194:THR:HG23	1.97	0.45
2:D:312:TYR:HA	2:D:381:SER:HA	1.98	0.45
1:C:201:ALA:HB3	1:C:267:PHE:CD2	2.52	0.45
2:D:333:LEU:HA	2:D:333:LEU:HD23	1.76	0.45
2:D:346:TRP:H	2:D:346:TRP:CD1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:237:THR:CG2	4:F:249:TYR:CD2	3.00	0.45
2:B:40:SER:HG	2:B:42:LEU:HB2	1.82	0.45
1:A:3:GLU:HB3	1:A:64:ARG:HD3	1.99	0.45
1:C:1:MET:HG3	1:C:131:GLY:HA3	1.98	0.45
1:C:18:ASN:ND2	1:C:78:VAL:HG22	2.31	0.45
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.98	0.45
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.99	0.45
1:C:247:ALA:C	1:C:248:LEU:HD23	2.42	0.45
2:B:265:LEU:N	2:B:265:LEU:HD23	2.32	0.45
1:A:115:ILE:HD13	1:A:152:LEU:HG	1.99	0.44
1:C:100:ALA:HB3	1:C:105:ARG:HD2	1.99	0.44
1:C:190:THR:HG23	1:C:191:THR:N	2.32	0.44
2:D:206:ASN:HA	2:D:209:LEU:HB2	1.98	0.44
2:D:226:ASP:C	2:D:228:ASN:N	2.74	0.44
4:F:283:ILE:HD11	4:F:321:VAL:HG11	1.98	0.44
1:A:286:LEU:N	1:A:286:LEU:HD22	2.32	0.44
1:C:271:THR:HG21	1:C:295:CYS:HA	1.99	0.44
2:D:269:MET:HE2	2:D:301:MET:SD	2.58	0.44
2:D:275:LEU:HA	2:D:275:LEU:HD23	1.66	0.44
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.98	0.44
1:A:262:TYR:CE1	1:A:346:TRP:CZ2	2.94	0.44
1:C:174:ALA:HB2	1:C:207:GLU:H	1.83	0.44
3:E:138:GLU:OE1	3:E:138:GLU:HA	2.17	0.44
4:F:240:LEU:O	4:F:245:ILE:HD11	2.18	0.44
4:F:255:ARG:HG2	4:F:256:TYR:N	2.33	0.44
1:C:156:ARG:HD2	1:C:156:ARG:HA	1.83	0.44
2:D:6:HIS:NE2	2:D:8:GLN:HB3	2.33	0.44
2:D:20:PHE:HB2	2:D:235:MET:SD	2.57	0.44
2:D:182:VAL:HG12	2:D:185:TYR:HD2	1.81	0.44
4:F:191:LEU:HD22	4:F:228:TYR:HB3	2.00	0.44
1:C:36:MET:SD	1:C:39:ASP:HB2	2.58	0.44
1:C:234:ILE:HG12	1:C:272:TYR:HB2	1.99	0.44
2:D:109:THR:OG1	2:D:110:GLU:N	2.50	0.44
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.47	0.44
4:F:200:ASP:HB2	4:F:241:THR:OG1	2.18	0.44
1:A:96:LYS:HG2	1:A:97:GLU:N	2.31	0.44
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.99	0.44
1:A:230:LEU:O	1:A:234:ILE:CD1	2.66	0.44
1:C:141:PHE:HD1	1:C:141:PHE:HA	1.71	0.44
2:D:78:VAL:O	2:D:84:GLY:HA3	2.18	0.44
2:B:31:ASP:C	2:B:33:THR:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:MET:HE3	2:B:375:ALA:CB	2.48	0.44
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.52	0.44
2:D:199:ASP:O	2:D:266:HIS:HB2	2.17	0.44
2:B:320:ARG:HA	2:B:356:CYS:O	2.18	0.44
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.99	0.44
2:D:105:LYS:HD3	2:D:411:GLU:CD	2.42	0.44
2:D:115:VAL:HG13	2:D:116:ASP:H	1.83	0.44
3:E:88:GLU:O	3:E:92:ASN:HB2	2.17	0.44
4:F:160:ILE:CG2	4:F:161:LEU:N	2.81	0.44
4:F:283:ILE:HD13	4:F:321:VAL:HG22	1.99	0.44
2:B:295:MET:HE1	2:B:375:ALA:HB1	1.97	0.44
2:B:298:SER:OG	2:B:307:PRO:HD2	2.18	0.44
2:D:63:PRO:HG2	2:D:87:PHE:HD1	1.82	0.43
2:D:209:LEU:HD23	2:D:230:LEU:HB2	1.98	0.43
2:D:305:CYS:SG	2:D:384[B]:ILE:HA	2.57	0.43
1:C:75:ILE:O	1:C:78:VAL:N	2.49	0.43
2:D:19:LYS:NZ	2:D:225:GLY:HA2	2.33	0.43
2:D:68:VAL:HA	2:D:93:VAL:O	2.19	0.43
2:D:352:LYS:HD3	2:D:352:LYS:HA	1.76	0.43
3:E:140:LYS:HD2	3:E:140:LYS:O	2.18	0.43
1:A:60:LYS:HD2	1:A:62:VAL:HG23	2.01	0.43
1:A:85:GLN:H	1:A:85:GLN:HG2	1.36	0.43
1:A:280:LYS:CE	1:A:283:HIS:ND1	2.80	0.43
1:C:156:ARG:HD3	3:E:101:LEU:HD11	1.98	0.43
1:C:187:SER:HB3	1:C:391:LEU:HD13	1.99	0.43
1:C:233:GLN:HG3	1:C:368:LEU:HD23	1.99	0.43
4:F:349:GLY:O	4:F:353[B]:VAL:HG13	2.18	0.43
2:B:69:ASP:OD2	2:B:74:THR:OG1	2.33	0.43
2:B:70:LEU:HD23	2:B:114:LEU:CD2	2.48	0.43
1:A:63:PRO:HG2	1:A:86:LEU:HD21	2.00	0.43
1:A:109:THR:O	1:A:110:ILE:CG1	2.66	0.43
1:C:401:LYS:HA	1:C:401:LYS:HD3	1.74	0.43
2:D:69:ASP:HB3	2:D:75:MET:CE	2.48	0.43
2:B:2:ARG:HA	2:B:131:CYS:O	2.19	0.43
2:B:120:ASP:OD1	2:B:123:ARG:NH2	2.51	0.43
1:A:49:PHE:CD1	1:A:49:PHE:C	2.96	0.43
1:C:139:HIS:CG	1:C:150:THR:HG21	2.54	0.43
2:D:291:LEU:HD11	2:D:373:MET:HB3	2.00	0.43
4:F:24:THR:C	4:F:26:GLN:H	2.26	0.43
4:F:234:GLN:O	4:F:234:GLN:CG	2.67	0.43
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:THR:O	2:B:400:ARG:HG2	2.19	0.43
1:A:12:ALA:CB	1:A:140:SER:HB3	2.49	0.43
1:C:355:ILE:HG13	8:C:504:A1EPQ:F62	2.08	0.43
2:D:220:THR:O	2:D:221:THR:CG2	2.67	0.43
1:A:71:GLU:HB3	1:A:98:ASP:HB3	2.00	0.43
1:A:76:ASP:HA	1:A:79:ARG:HG2	2.00	0.43
1:A:97:GLU:HG2	2:B:131:CYS:SG	2.59	0.43
1:C:30:ILE:HD11	1:C:36:MET:CE	2.49	0.43
2:D:180:THR:O	2:D:183:GLU:HG3	2.18	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.01	0.43
2:D:190:SER:O	2:D:193:GLN:HB2	2.18	0.43
3:E:101:LEU:HD23	3:E:101:LEU:HA	1.85	0.43
4:F:22:LEU:C	4:F:24:THR:N	2.76	0.43
4:F:167:SER:O	4:F:168:GLU:HB2	2.18	0.43
4:F:225:SER:CB	4:F:250:SER:HA	2.49	0.43
1:A:3:GLU:HB3	1:A:64:ARG:NE	2.34	0.42
2:D:133:GLN:O	2:D:164:ARG:HD3	2.19	0.42
2:D:188:THR:HG22	2:D:421:ALA:HB1	1.99	0.42
2:D:372:LYS:O	2:D:373:MET:HG2	2.19	0.42
2:B:112:ALA:O	2:B:113:GLU:C	2.61	0.42
1:A:415:GLU:O	1:A:418:PHE:HB2	2.19	0.42
1:C:86:LEU:HD12	1:C:86:LEU:HA	1.69	0.42
1:C:317:LEU:C	1:C:318:LEU:HD12	2.45	0.42
1:C:324:VAL:O	1:C:325:PRO:C	2.62	0.42
2:D:343:PHE:CE2	2:D:351:VAL:CG2	3.03	0.42
4:F:205:VAL:HG11	4:F:291:ILE:CG2	2.49	0.42
4:F:233:PHE:HA	4:F:239:HIS:CD2	2.54	0.42
1:A:258:ASN:OD1	1:A:352:LYS:HE2	2.19	0.42
1:C:271:THR:HG22	1:C:295:CYS:HA	2.01	0.42
2:D:66:ILE:CD1	2:D:122:VAL:HA	2.49	0.42
3:E:22:VAL:HG13	3:E:22:VAL:O	2.20	0.42
4:F:38:ASN:O	4:F:60:GLN:HA	2.18	0.42
1:A:261:PRO:HG2	1:A:313:MET:HB3	2.01	0.42
1:C:265:ILE:HG23	1:C:432:TYR:CZ	2.55	0.42
2:D:88:ARG:O	2:D:88:ARG:HG2	2.20	0.42
2:D:142:GLY:O	2:D:186:ASN:ND2	2.52	0.42
2:D:286:LEU:HD23	2:D:286:LEU:N	2.26	0.42
2:D:402:LYS:O	2:D:403:ALA:C	2.63	0.42
4:F:2:TYR:CE2	4:F:359:PHE:HB3	2.54	0.42
2:B:215:ARG:O	2:B:216:THR:C	2.62	0.42
1:C:383:ALA:C	1:C:385:ALA:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:CYS:SG	2:D:227:LEU:HD23	2.58	0.42
2:D:404:PHE:CD2	2:D:404:PHE:N	2.87	0.42
4:F:198:LYS:HB2	4:F:198:LYS:HE2	1.83	0.42
1:A:5:ILE:HB	1:A:135:PHE:HD1	1.84	0.42
1:C:368:LEU:HD12	1:C:368:LEU:HA	1.87	0.42
4:F:55:GLU:OE1	4:F:55:GLU:HA	2.19	0.42
4:F:135:TYR:HE2	4:F:166:ALA:HB2	1.85	0.42
2:B:241:CYS:O	2:B:250:ALA:HA	2.20	0.42
2:B:403:ALA:O	2:B:404:PHE:HB2	2.20	0.42
1:C:93:ILE:HD11	1:C:121:ARG:CG	2.43	0.42
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.00	0.42
1:C:97:GLU:HB2	2:D:131:CYS:SG	2.60	0.42
2:D:104:ALA:CB	2:D:413:MET:CE	2.93	0.42
3:E:119:MET:O	3:E:123:LEU:HG	2.19	0.42
1:A:117:LEU:HD12	1:A:117:LEU:O	2.19	0.42
1:C:233:GLN:HA	1:C:233:GLN:OE1	2.20	0.42
1:A:187:SER:CB	1:A:391:LEU:HD21	2.49	0.42
1:A:436:GLY:O	1:A:437:VAL:C	2.62	0.42
8:C:504:A1EPQ:N11	8:C:504:A1EPQ:O29	2.53	0.42
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.54	0.42
2:D:172:MET:HE3	2:D:172:MET:HB3	1.65	0.42
2:D:217:LEU:HD21	2:D:276:THR:O	2.20	0.42
2:B:297:ASP:HA	2:B:308:ARG:NH2	2.28	0.42
1:C:108:TYR:HB3	3:E:105:MET:SD	2.59	0.42
2:B:48:ARG:HB2	2:B:243:ARG:O	2.19	0.42
1:A:76:ASP:OD1	1:A:79:ARG:HD3	2.20	0.41
1:C:36:MET:O	1:C:37:PRO:C	2.63	0.41
1:C:41:THR:CB	1:C:44:GLY:O	2.68	0.41
2:D:109:THR:O	2:D:113:GLU:HG3	2.20	0.41
3:E:100:LYS:O	3:E:104:LYS:HB2	2.20	0.41
3:E:103:GLN:O	3:E:103:GLN:HG2	2.19	0.41
2:B:168[A]:THR:HG21	2:B:198:THR:HG21	2.01	0.41
1:A:131:GLY:O	1:A:132:LEU:C	2.63	0.41
1:A:234:ILE:HG21	1:A:302:MET:HE2	2.02	0.41
1:C:9:VAL:HG22	1:C:68[B]:VAL:HG13	2.02	0.41
2:B:325:MET:HE2	2:B:325:MET:HB3	1.74	0.41
2:B:70:LEU:HD23	2:B:114:LEU:HD22	2.01	0.41
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.36	0.41
1:A:76:ASP:HA	1:A:79:ARG:CD	2.50	0.41
1:C:39:ASP:OD1	1:C:41:THR:OG1	2.39	0.41
2:D:312:TYR:O	2:D:344:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:206:LEU:HD21	4:F:353[B]:VAL:HG22	2.02	0.41
1:A:307:PRO:HA	1:A:383:ALA:HB2	2.01	0.41
1:C:91:GLN:O	1:C:92:LEU:HD23	2.21	0.41
2:D:72:PRO:HD3	2:D:95:GLY:O	2.20	0.41
2:D:114:LEU:O	2:D:115:VAL:C	2.62	0.41
4:F:14:TYR:HA	4:F:17:VAL:CG2	2.45	0.41
1:A:84:ARG:HG2	1:A:85:GLN:N	2.34	0.41
1:C:318:LEU:N	1:C:318:LEU:HD12	2.35	0.41
4:F:190:LEU:H	4:F:322:ASP:HA	1.84	0.41
4:F:322:ASP:OD1	4:F:322:ASP:C	2.63	0.41
1:C:270:ALA:HA	1:C:377:MET:O	2.21	0.41
2:D:288:VAL:CG1	2:D:327:GLU:HG2	2.51	0.41
4:F:230:SER:O	4:F:231:ALA:HB3	2.21	0.41
1:A:30:ILE:HG12	1:A:36:MET:HB2	2.02	0.41
1:A:149:PHE:O	1:A:152:LEU:HB3	2.21	0.41
1:A:413:MET:CE	1:A:418:PHE:CE2	3.04	0.41
2:D:3:GLU:HG2	2:D:64:ARG:NH2	2.36	0.41
2:D:67:LEU:N	2:D:67:LEU:HD12	2.36	0.41
2:D:82:PRO:O	2:D:83:PHE:HB2	2.21	0.41
2:D:214:PHE:HA	2:D:219:LEU:O	2.21	0.41
2:B:248:LEU:O	2:B:249:ASN:C	2.64	0.41
1:A:5:ILE:HG12	1:A:132:LEU:CD1	2.51	0.41
1:A:35:GLN:HA	1:A:35:GLN:NE2	2.35	0.41
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.86	0.41
1:A:126:ALA:O	1:A:129:CYS:HB2	2.20	0.41
1:A:153:LEU:HD12	1:A:153:LEU:C	2.44	0.41
1:C:116:ASP:O	1:C:117:LEU:C	2.63	0.41
2:D:57:THR:HG22	2:D:58:GLY:N	2.36	0.41
2:D:237:GLY:CA	2:D:376:THR:HG21	2.40	0.41
2:D:274:PRO:HD2	2:D:371:LEU:CD1	2.34	0.41
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.03	0.41
4:F:66:ARG:O	4:F:302:ILE:HG22	2.20	0.41
1:A:93:ILE:HD11	1:A:121:ARG:CB	2.51	0.41
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.80	0.41
1:C:39:ASP:OD2	1:C:55:GLU:OE2	2.39	0.41
1:C:132:LEU:HD12	1:C:132:LEU:HA	1.86	0.41
2:D:12:CYS:O	2:D:16:ILE:HG23	2.21	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.56	0.41
2:D:301:MET:HA	2:D:301:MET:HE2	2.03	0.41
1:A:54:SER:HA	1:A:64:ARG:HH12	1.86	0.40
4:F:5:VAL:HB	4:F:32:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:234:GLN:O	4:F:234:GLN:HG3	2.21	0.40
2:D:107:HIS:O	2:D:152:LEU:HD22	2.21	0.40
2:D:174:SER:C	2:D:176:LYS:H	2.30	0.40
3:E:140:LYS:C	3:E:140:LYS:CD	2.94	0.40
4:F:163:SER:HB3	4:F:169:LEU:HD13	2.02	0.40
1:A:54:SER:O	1:A:61:HIS:HA	2.21	0.40
1:A:90:GLU:O	1:A:121:ARG:CD	2.70	0.40
2:D:42:LEU:H	2:D:42:LEU:CD2	2.34	0.40
2:D:248:LEU:O	2:D:249:ASN:C	2.64	0.40
2:D:403:ALA:HB1	2:D:404:PHE:HD2	1.86	0.40
4:F:100:ILE:O	4:F:179:VAL:HG13	2.20	0.40
4:F:278:THR:HG22	4:F:279:LEU:N	2.36	0.40
2:B:124:LYS:HB3	2:B:124:LYS:HE2	1.82	0.40
2:B:136:GLN:O	2:B:136:GLN:HG3	2.22	0.40
1:C:114:ILE:HG12	1:C:114:ILE:O	2.21	0.40
2:D:103:TRP:O	2:D:104:ALA:C	2.65	0.40
2:D:233:ALA:HB1	2:D:272:PHE:CE2	2.56	0.40
2:D:251:ASP:OD2	2:D:254:LYS:HG3	2.22	0.40
2:B:310:GLY:HA2	2:B:436:GLN:NE2	2.37	0.40
1:A:182:VAL:O	1:A:185:TYR:HB2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:SER:OG	4:F:292:ARG:NH2[3_545]	2.05	0.15
1:C:282:TYR:OH	2:B:411:GLU:OE1[4_455]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/450 (99%)	398 (89%)	41 (9%)	7 (2%)	7	17
1	C	445/450 (99%)	412 (93%)	29 (6%)	4 (1%)	14	28
2	B	428/445 (96%)	401 (94%)	25 (6%)	2 (0%)	24	42
2	D	424/445 (95%)	366 (86%)	51 (12%)	7 (2%)	7	16
3	E	116/143 (81%)	110 (95%)	6 (5%)	0	100	100
4	F	323/384 (84%)	293 (91%)	24 (7%)	6 (2%)	6	14
All	All	2182/2317 (94%)	1980 (91%)	176 (8%)	26 (1%)	11	22

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ILE
1	C	41	THR
4	F	42	GLY
1	C	322	ASP
2	D	64	ARG
2	D	133	GLN
4	F	23	ALA
4	F	32	LYS
2	B	215	ARG
2	D	79	ARG
2	D	403	ALA
1	A	346	TRP
1	C	284	GLU
2	D	215	ARG
2	D	304	ALA
1	A	57	GLY
1	C	109	THR
1	A	128	GLN
4	F	275[A]	LEU
4	F	275[B]	LEU
4	F	25	GLY
1	A	68[A]	VAL
1	A	68[B]	VAL
1	A	114	ILE
2	B	32	PRO
2	D	78	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/378 (100%)	349 (92%)	29 (8%)	12	25
1	C	378/378 (100%)	358 (95%)	20 (5%)	20	42
2	B	369/383 (96%)	350 (95%)	19 (5%)	21	43
2	D	369/383 (96%)	347 (94%)	22 (6%)	17	36
3	E	108/127 (85%)	96 (89%)	12 (11%)	6	12
4	F	303/342 (89%)	278 (92%)	25 (8%)	10	22
All	All	1905/1991 (96%)	1778 (93%)	127 (7%)	16	31

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	67	PHE
1	A	68[A]	VAL
1	A	68[B]	VAL
1	A	71	GLU
1	A	82	THR
1	A	84	ARG
1	A	94	THR
1	A	118	VAL
1	A	121	ARG
1	A	122	ILE
1	A	124	LYS
1	A	128	GLN
1	A	163	LYS
1	A	165	SER
1	A	176	GLN
1	A	179	THR
1	A	181	VAL
1	A	214	ARG
1	A	251	ASP
1	A	253	THR
1	A	257	THR

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Mol	Chain	Res	Type
1	A	315[A]	CYS
1	A	315[B]	CYS
1	A	334	THR
1	A	336	LYS
1	A	340	SER
1	A	363	VAL
1	A	419	SER
1	C	85	GLN
1	C	108	TYR
1	C	109	THR
1	C	112	LYS
1	C	117	LEU
1	C	141	PHE
1	C	159	VAL
1	C	170	SER
1	C	183	GLU
1	C	245	ASP
1	C	286	LEU
1	C	318	LEU
1	C	362	VAL
1	C	363[A]	VAL
1	C	363[B]	VAL
1	C	368	LEU
1	C	379	SER
1	C	401	LYS
1	C	430	LYS
1	C	439	SER
2	D	5	VAL
2	D	16	ILE
2	D	25	SER
2	D	26	ASP
2	D	62	VAL
2	D	88	ARG
2	D	90	ASP
2	D	121	VAL
2	D	128	SER
2	D	179	ASP
2	D	180	THR
2	D	182	VAL
2	D	195	VAL
2	D	248	LEU
2	D	275	LEU

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Mol	Chain	Res	Type
2	D	305	CYS
2	D	344	VAL
2	D	345	GLU
2	D	376	THR
2	D	387	LEU
2	D	409	THR
2	D	441	ASP
3	E	7	GLU
3	E	16	SER
3	E	19	SER
3	E	28	SER
3	E	49	GLU
3	E	58	GLU
3	E	67	GLU
3	E	87	ILE
3	E	92	ASN
3	E	107	SER
3	E	128	LYS
3	E	140	LYS
4	F	3	THR
4	F	9	GLU
4	F	12	SER
4	F	26	GLN
4	F	47	LEU
4	F	84	SER
4	F	130	VAL
4	F	162	ILE
4	F	171	ASP
4	F	180	HIS
4	F	188	LYS
4	F	192	LEU
4	F	197	ARG
4	F	201	ILE
4	F	239	HIS
4	F	241	THR
4	F	247	LYS
4	F	275[A]	LEU
4	F	275[B]	LEU
4	F	284[A]	LEU
4	F	284[B]	LEU
4	F	323	GLU
4	F	330	ILE

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Mol	Chain	Res	Type
4	F	356	SER
4	F	373	SER
2	B	25	SER
2	B	39	ASP
2	B	74	THR
2	B	117	SER
2	B	137	LEU
2	B	168[A]	THR
2	B	168[B]	THR
2	B	238	VAL
2	B	278	ARG
2	B	288	VAL
2	B	330	GLU
2	B	334	ASN
2	B	336	GLN
2	B	369	ARG
2	B	371	LEU
2	B	389	LYS
2	B	405	LEU
2	B	430	SER
2	B	434	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	50	ASN
1	A	61	HIS
1	A	91	GLN
1	A	256	GLN
1	A	285	GLN
1	A	309	HIS
1	A	406	HIS
1	C	11	GLN
1	C	18	ASN
1	C	309	HIS
1	C	329	ASN
2	D	133	GLN
2	D	228	ASN
2	D	247	GLN
2	D	300	ASN
3	E	12	ASN

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Mol	Chain	Res	Type
3	E	84	GLN
3	E	111	ASN
3	E	115	HIS
4	F	34	ASN
4	F	243	HIS
4	F	286	GLN
2	B	8	GLN
2	B	136	GLN
2	B	167	ASN
2	B	294	GLN
2	B	349	ASN
2	B	385	GLN
2	B	433	GLN
2	B	434	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GDP	B	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
9	GDP	D	501	-	29,30,30	1.94	5 (17%)	45,47,47	2.64	18 (40%)
8	A1EPQ	C	504	-	70,71,71	5.08	32 (45%)	88,115,115	2.73	34 (38%)
5	GTP	A	501	7	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
5	GTP	C	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.63	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	502	-	-	0/16/32/32	0/3/3/3
9	GDP	D	501	-	-	0/16/32/32	0/3/3/3
8	A1EPQ	C	504	-	-	4/42/133/133	0/7/9/9
5	GTP	A	501	7	-	4/22/38/38	0/3/3/3
5	GTP	C	501	-	-	3/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	504	A1EPQ	C20-C15	16.47	1.58	1.39
8	C	504	A1EPQ	C08-C09	13.31	1.55	1.32
8	C	504	A1EPQ	C16-C15	11.75	1.56	1.39
8	C	504	A1EPQ	C20-N02	11.56	1.59	1.39
8	C	504	A1EPQ	C49-C50	10.79	1.56	1.39
8	C	504	A1EPQ	C19-C18	10.68	1.57	1.38
8	C	504	A1EPQ	C16-C17	10.10	1.53	1.39
8	C	504	A1EPQ	C18-C17	9.33	1.57	1.39
8	C	504	A1EPQ	C13-C12	8.89	1.68	1.52
8	C	504	A1EPQ	C19-C20	8.69	1.53	1.39
9	D	501	GDP	C5-N7	-6.96	1.25	1.39
8	C	504	A1EPQ	C45-C46	6.77	1.55	1.40
8	C	504	A1EPQ	C49-C48	6.29	1.48	1.37
8	C	504	A1EPQ	C46-C47	5.90	1.50	1.39
8	C	504	A1EPQ	C07-C08	5.79	1.62	1.51
8	C	504	A1EPQ	C14-C04	5.45	1.74	1.55
8	C	504	A1EPQ	C48-C47	5.36	1.47	1.37
8	C	504	A1EPQ	C07-C21	-5.08	1.42	1.53
8	C	504	A1EPQ	C21-N11	5.08	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	504	A1EPQ	C05-C06	-4.92	1.40	1.54
8	C	504	A1EPQ	O60-C58	4.91	1.42	1.33
8	C	504	A1EPQ	C43-C44	4.86	1.58	1.51
8	C	504	A1EPQ	C14-C15	-4.79	1.44	1.51
9	D	501	GDP	O6-C6	4.73	1.32	1.23
8	C	504	A1EPQ	O27-C25	4.59	1.41	1.33
8	C	504	A1EPQ	C10-C09	4.48	1.60	1.49
8	C	504	A1EPQ	O30-C06	3.87	1.52	1.44
8	C	504	A1EPQ	C04-N02	-3.74	1.39	1.47
8	C	504	A1EPQ	C05-C25	3.61	1.61	1.52
8	C	504	A1EPQ	C45-C44	-3.28	1.38	1.44
9	B	502	GDP	C5-C4	3.20	1.47	1.38
8	C	504	A1EPQ	O34-C18	2.62	1.41	1.37
8	C	504	A1EPQ	C52-C44	2.47	1.40	1.37
9	D	501	GDP	C4-N3	2.45	1.39	1.34
9	B	502	GDP	C6-N1	-2.43	1.34	1.38
8	C	504	A1EPQ	O30-C31	2.41	1.40	1.35
9	D	501	GDP	C2-N2	-2.38	1.28	1.34
8	C	504	A1EPQ	C54-C37	-2.37	1.49	1.52
5	A	501	GTP	C2-N3	2.20	1.38	1.33
5	C	501	GTP	C2-N3	2.17	1.38	1.33
9	D	501	GDP	C8-N9	2.10	1.42	1.37
9	B	502	GDP	C5-N7	-2.06	1.34	1.39

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	504	A1EPQ	C13-C14-C15	-12.57	89.49	112.36
8	C	504	A1EPQ	C14-C21-C07	-7.60	112.56	118.20
8	C	504	A1EPQ	C13-C14-C04	6.81	125.37	112.17
9	D	501	GDP	C4-C5-N7	6.75	121.36	110.67
9	D	501	GDP	N2-C2-N1	6.24	129.92	116.76
9	B	502	GDP	C5-C4-N3	-6.22	118.48	128.39
8	C	504	A1EPQ	C05-C04-C14	-5.99	101.82	114.18
9	D	501	GDP	N1-C2-N3	-5.90	112.53	123.32
5	C	501	GTP	C5-C4-N3	-5.47	119.69	128.39
9	D	501	GDP	O6-C6-N1	-5.21	110.32	120.11
9	B	502	GDP	C2-N3-C4	5.04	120.98	112.30
5	A	501	GTP	C5-C4-N3	-4.99	120.45	128.39
5	C	501	GTP	C2-N3-C4	4.91	120.76	112.30
8	C	504	A1EPQ	C21-C07-C08	4.90	113.16	108.27
8	C	504	A1EPQ	O34-C18-C17	4.72	121.27	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	4.62	120.26	112.30
9	B	502	GDP	N9-C4-N3	4.61	135.17	125.95
9	D	501	GDP	C3'-C2'-C1'	4.40	109.80	101.46
8	C	504	A1EPQ	C07-C08-C09	-4.29	114.76	123.88
9	D	501	GDP	C5-C4-N9	-4.12	98.28	105.66
8	C	504	A1EPQ	C16-C15-C20	-3.91	117.03	120.29
8	C	504	A1EPQ	C07-C21-N11	3.88	119.91	111.72
9	D	501	GDP	C2-N3-C4	3.87	118.96	112.30
8	C	504	A1EPQ	C54-N41-C40	3.83	116.06	110.87
8	C	504	A1EPQ	O27-C25-C05	3.77	118.42	112.21
8	C	504	A1EPQ	C22-C07-C08	-3.70	103.58	107.99
8	C	504	A1EPQ	C50-C45-C46	3.64	121.28	117.70
5	C	501	GTP	N9-C4-N3	3.63	133.21	125.95
8	C	504	A1EPQ	C16-C15-C14	3.48	134.95	129.01
9	D	501	GDP	C6-C5-C4	-3.48	113.60	118.83
9	D	501	GDP	N9-C4-N3	3.46	132.87	125.95
9	D	501	GDP	O6-C6-C5	3.44	135.61	126.53
8	C	504	A1EPQ	O30-C31-C32	3.39	117.13	111.09
9	D	501	GDP	C2-N1-C6	3.30	131.11	125.11
8	C	504	A1EPQ	C19-C18-C17	-3.22	118.79	122.11
5	A	501	GTP	N9-C4-N3	3.20	132.35	125.95
9	B	502	GDP	C6-C5-N7	3.18	136.07	130.29
9	D	501	GDP	C1'-N9-C4	-3.09	117.34	126.49
8	C	504	A1EPQ	C35-O34-C18	-3.07	113.02	117.51
5	C	501	GTP	C2-N1-C6	-2.99	119.69	125.11
8	C	504	A1EPQ	C43-C44-C45	-2.97	115.86	123.91
9	D	501	GDP	C6-C5-N7	-2.97	124.89	130.29
9	D	501	GDP	O4'-C1'-N9	-2.90	101.79	108.36
5	A	501	GTP	C2-N1-C6	-2.89	119.86	125.11
8	C	504	A1EPQ	C10-C09-C08	-2.83	118.72	123.13
8	C	504	A1EPQ	C28-O27-C25	-2.82	111.28	115.91
8	C	504	A1EPQ	C04-C05-C25	-2.73	102.52	110.02
5	A	501	GTP	N9-C8-N7	-2.69	108.42	113.40
8	C	504	A1EPQ	C16-C17-C18	2.68	120.61	116.80
9	B	502	GDP	C4-C5-N7	-2.57	106.59	110.67
8	C	504	A1EPQ	O29-C05-C25	2.54	112.67	106.57
5	C	501	GTP	C5-C6-N1	2.54	119.71	113.25
5	A	501	GTP	C8-N7-C5	2.53	108.76	104.26
5	A	501	GTP	C5-C6-N1	2.51	119.65	113.25
8	C	504	A1EPQ	F63-C48-C47	2.51	121.72	118.32
9	B	502	GDP	C3'-C2'-C1'	2.50	106.19	101.46
5	C	501	GTP	C8-N7-C5	2.46	108.64	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N9-C8-N7	-2.43	108.89	113.40
5	C	501	GTP	O6-C6-C5	-2.42	120.13	126.53
5	A	501	GTP	O6-C6-C5	-2.42	120.15	126.53
9	D	501	GDP	O2'-C2'-C3'	-2.41	104.10	111.82
8	C	504	A1EPQ	O34-C18-C19	-2.40	119.94	124.08
8	C	504	A1EPQ	C14-C04-N02	2.36	109.86	105.38
8	C	504	A1EPQ	C15-C14-C21	2.34	123.04	115.26
8	C	504	A1EPQ	O27-C25-O26	-2.25	120.09	123.95
9	D	501	GDP	N9-C8-N7	-2.24	109.24	113.40
9	D	501	GDP	C1'-N9-C8	2.21	133.02	126.73
5	C	501	GTP	C3'-C2'-C1'	2.20	105.62	101.46
8	C	504	A1EPQ	C39-C38-C37	2.16	115.86	109.98
9	B	502	GDP	O6-C6-C5	-2.12	120.95	126.53
5	A	501	GTP	C3'-C2'-C1'	2.08	105.39	101.46
9	D	501	GDP	N2-C2-N3	-2.07	115.62	119.67
8	C	504	A1EPQ	O59-C58-C53	-2.05	119.93	124.81
8	C	504	A1EPQ	C50-N51-C52	-2.03	106.24	109.06
8	C	504	A1EPQ	O60-C58-O59	2.03	127.45	123.95
8	C	504	A1EPQ	C61-O60-C58	2.03	119.24	115.91
8	C	504	A1EPQ	C15-C14-C04	2.01	105.24	102.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

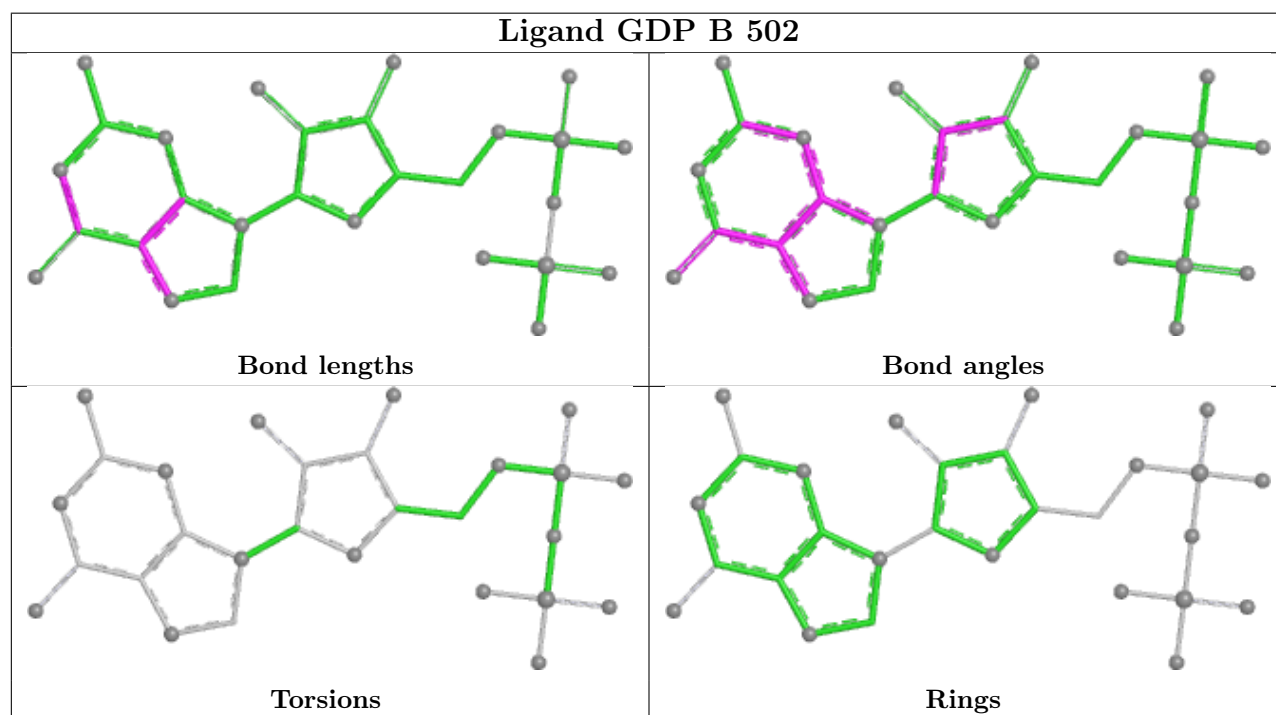
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
8	C	504	A1EPQ	C38-C39-C55-C56
8	C	504	A1EPQ	C40-C39-C55-C56
8	C	504	A1EPQ	O57-C39-C55-C56
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C2'-C1'-N9-C4
5	C	501	GTP	C2'-C1'-N9-C8
8	C	504	A1EPQ	N41-C42-C43-C44

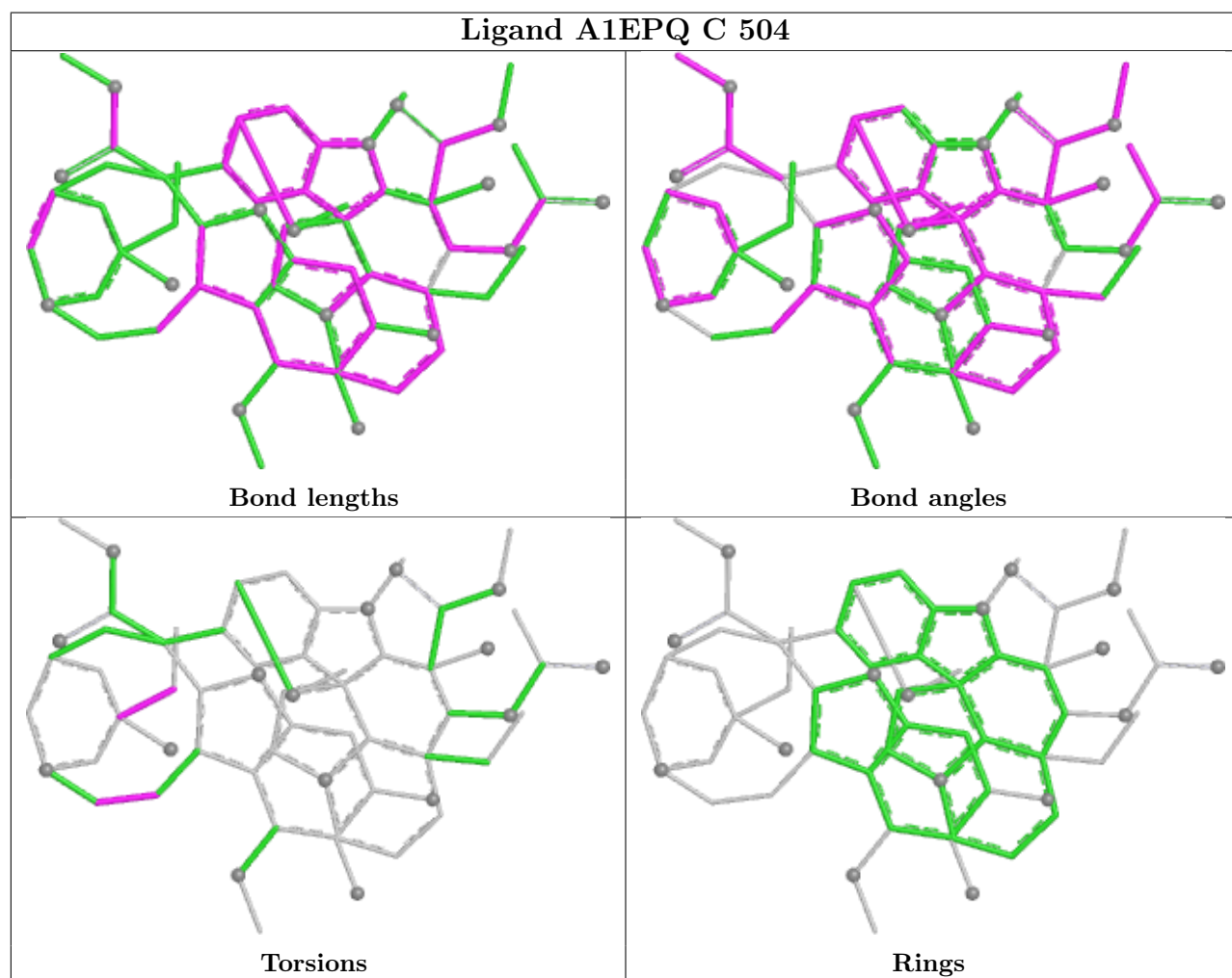
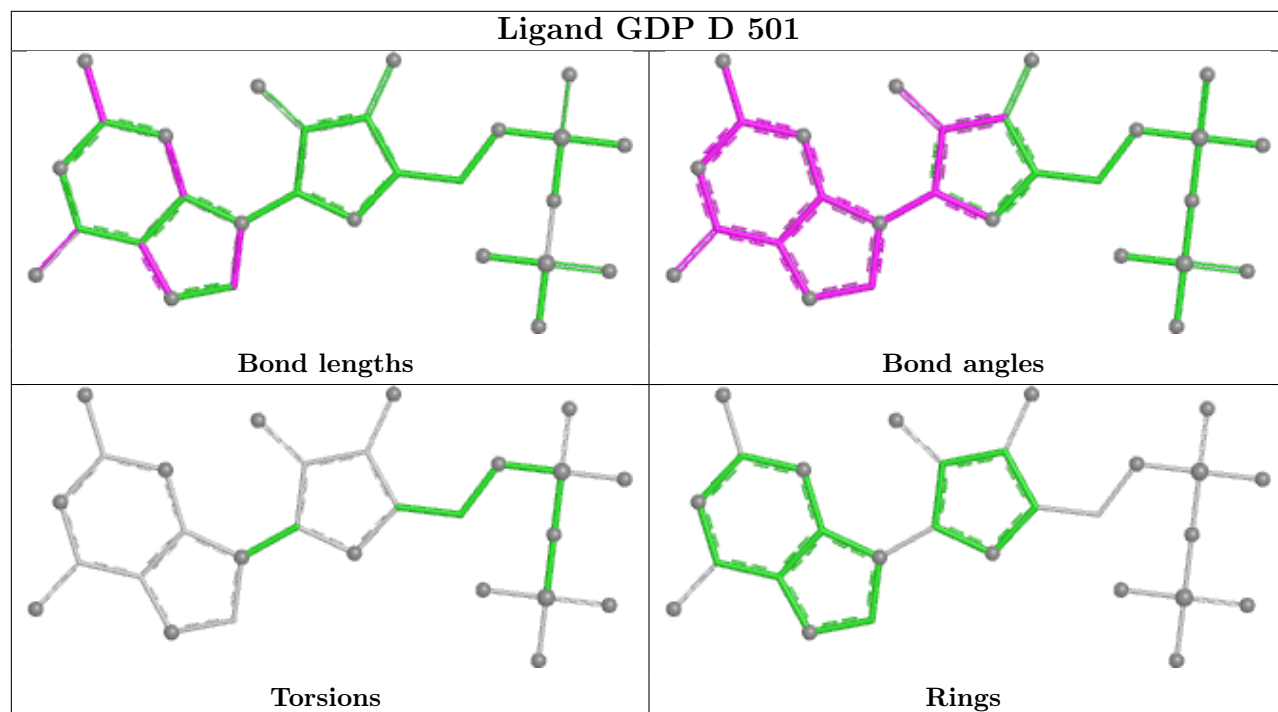
There are no ring outliers.

1 monomer is involved in 4 short contacts:

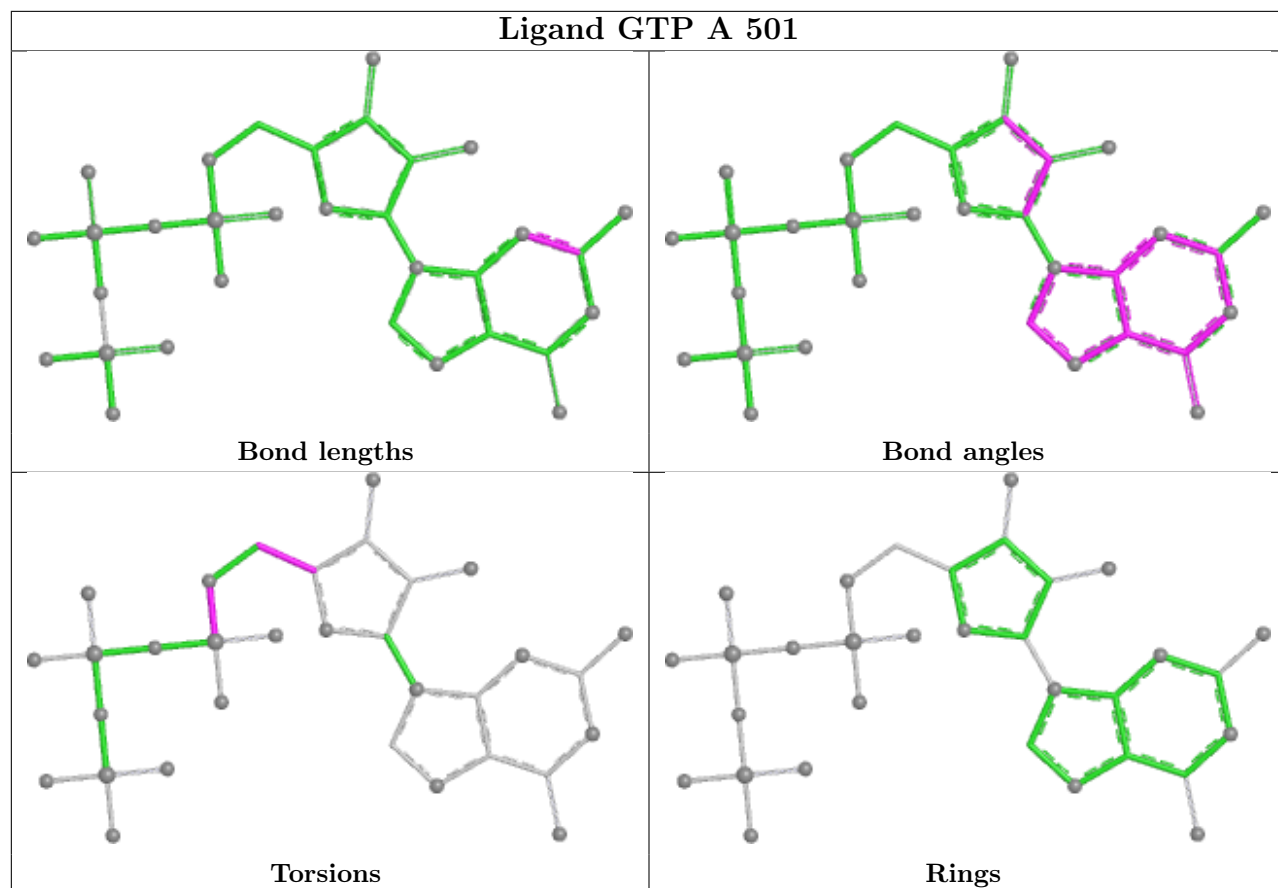
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	504	A1EPQ	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

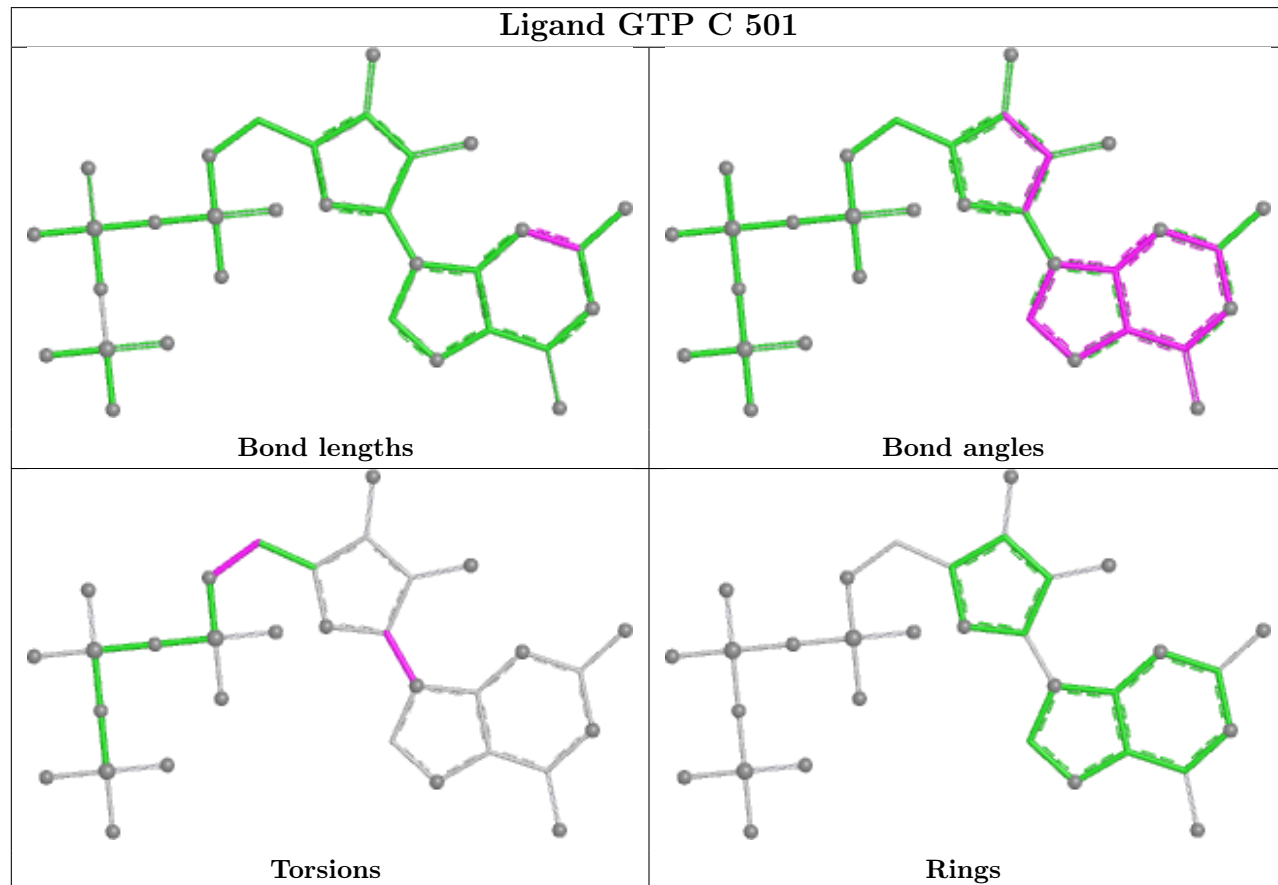




Ligand GTP A 501



Ligand GTP C 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/450 (97%)	-0.30	3 (0%) 84 80	17, 35, 60, 89	9 (2%)
1	C	440/450 (97%)	-0.45	3 (0%) 84 80	12, 28, 49, 74	7 (1%)
2	B	428/445 (96%)	-0.52	4 (0%) 81 76	13, 28, 55, 79	5 (1%)
2	D	424/445 (95%)	0.24	14 (3%) 49 40	19, 50, 79, 90	6 (1%)
3	E	120/143 (83%)	0.04	4 (3%) 49 40	27, 49, 74, 85	0
4	F	331/384 (86%)	0.32	22 (6%) 24 18	23, 51, 97, 118	4 (1%)
All	All	2182/2317 (94%)	-0.16	50 (2%) 61 52	12, 38, 76, 118	31 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	250	SER	4.4
4	F	233	PHE	4.2
1	C	440	VAL	3.8
4	F	331	GLU	3.7
2	D	403	ALA	3.7
4	F	130	VAL	3.7
4	F	362	ALA	3.6
4	F	180	HIS	3.3
1	A	437	VAL	3.3
2	D	228	ASN	3.3
2	D	144	GLY	3.3
2	D	143	GLY	3.3
4	F	170	LEU	3.2
4	F	247	LYS	3.1
2	D	1	MET	3.0
4	F	176	GLN	2.9
4	F	125	THR	2.8
2	B	1	MET	2.8
3	E	140	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	285	ALA	2.8
4	F	231	ALA	2.8
2	B	280	SER	2.7
1	A	282	TYR	2.7
3	E	23	ILE	2.6
4	F	178	GLN	2.6
2	D	304	ALA	2.6
4	F	173	ILE	2.5
4	F	144	GLY	2.5
1	C	283	HIS	2.4
2	D	180	THR	2.4
4	F	137	ARG	2.4
1	C	46	ASP	2.3
2	D	369	ARG	2.3
2	D	272	PHE	2.2
4	F	103	THR	2.2
4	F	177	GLY	2.2
2	B	438	ALA	2.2
3	E	6	MET	2.2
2	D	276	THR	2.2
2	B	283	TYR	2.2
3	E	28	SER	2.2
4	F	249	TYR	2.1
4	F	149	ALA	2.1
4	F	44	ARG	2.1
4	F	179	VAL	2.1
1	A	41	THR	2.1
2	D	82	PRO	2.1
2	D	181	VAL	2.0
2	D	440	ALA	2.0
4	F	372	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

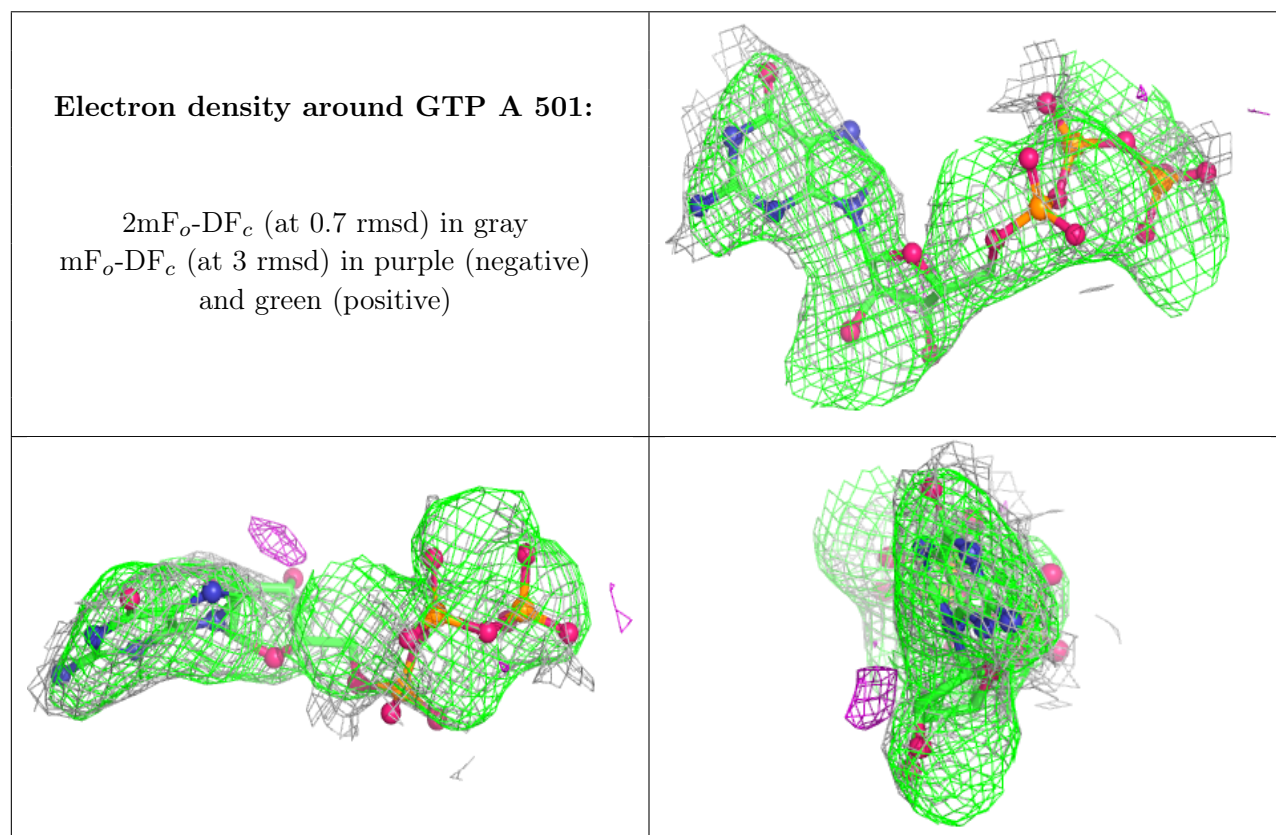
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

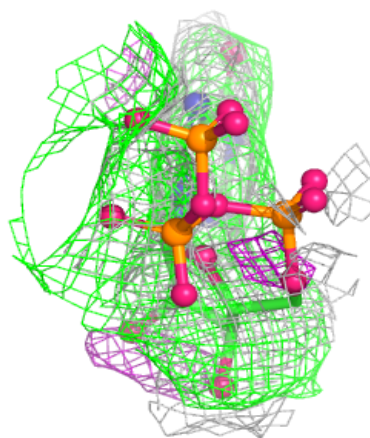
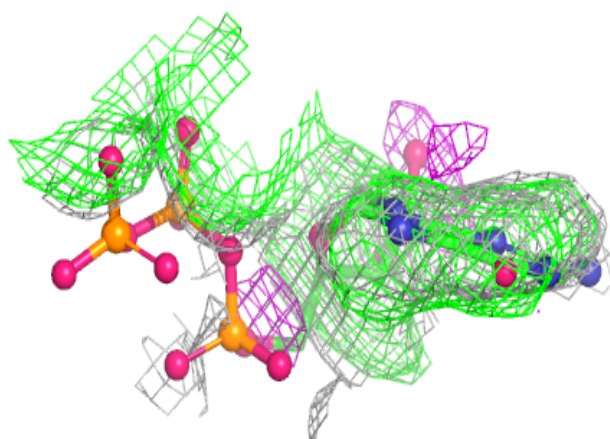
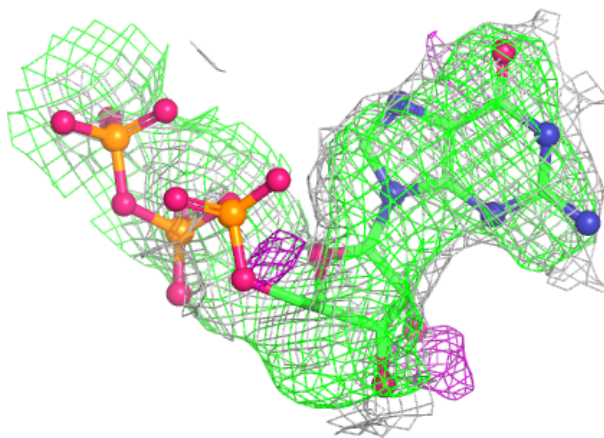
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	22,26,28,30	32
5	GTP	C	501	32/32	-	-	20,25,28,30	32
6	CA	A	502	1/1	-	-	56,56,56,56	1
6	CA	C	503	1/1	-	-	44,44,44,44	1
7	MG	C	502	1/1	-	-	22,22,22,22	1
7	MG	B	501	1/1	-	-	26,26,26,26	1
8	A1EPQ	C	504	63/63	0.95	0.09	19,30,38,54	0
9	GDP	D	501	28/28	-	-	53,56,58,59	28
9	GDP	B	502	28/28	-	-	17,19,20,22	28

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



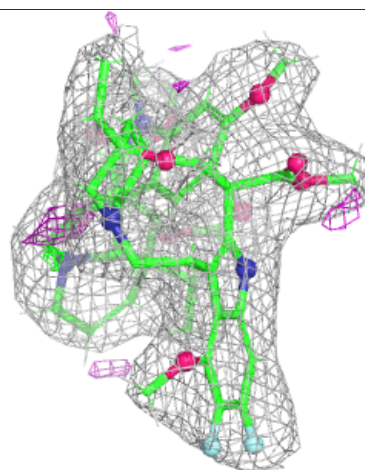
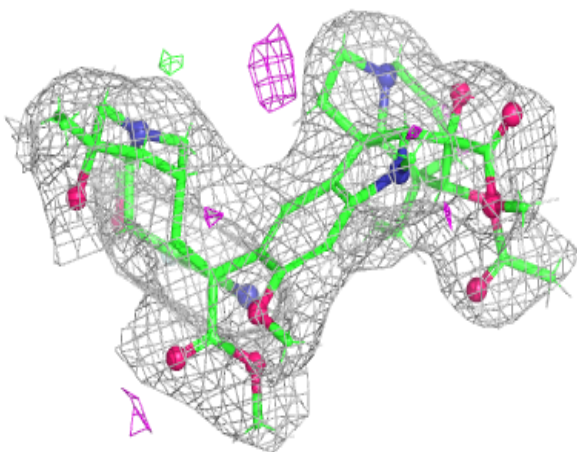
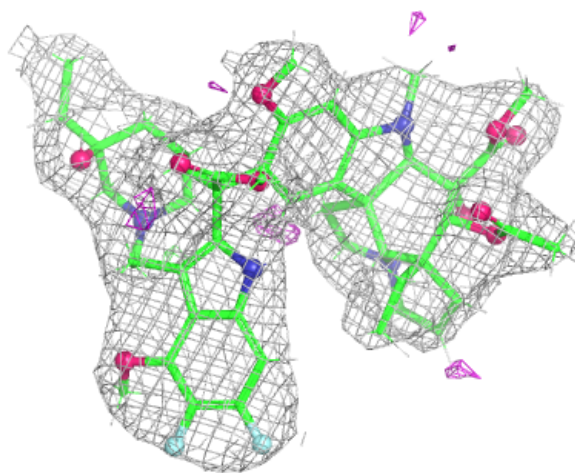
Electron density around GTP C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



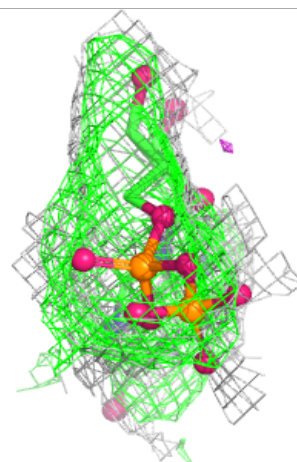
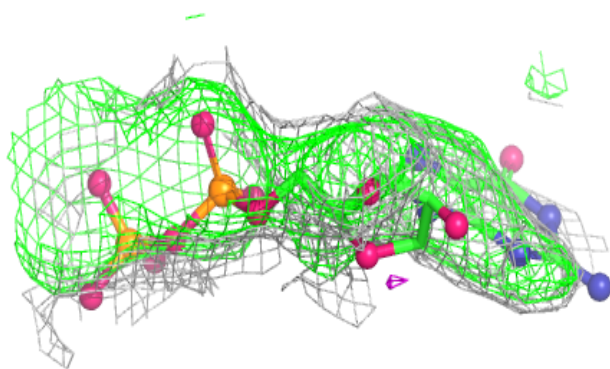
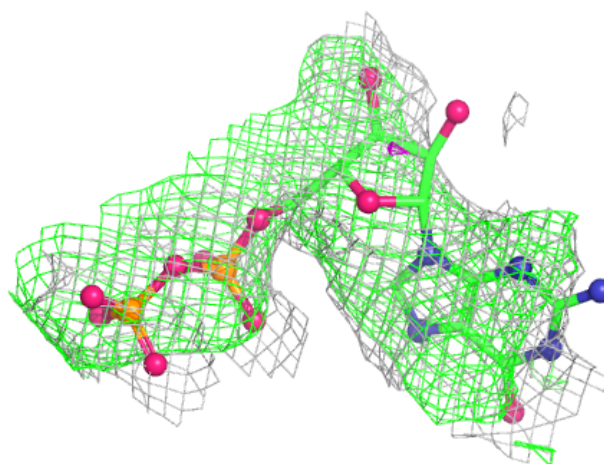
Electron density around A1EPQ C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



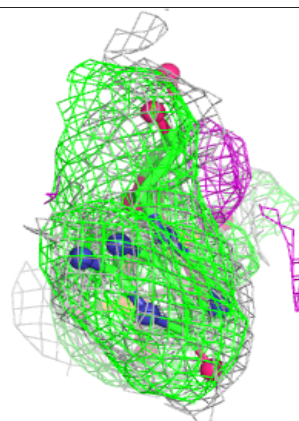
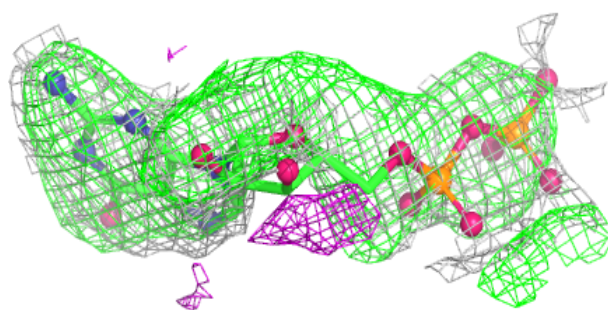
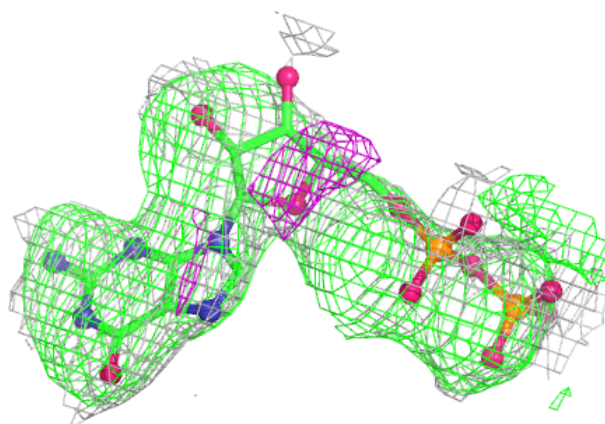
Electron density around GDP D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.